

**BINARY SOLUTION MODEL FOR
COMPUTATION OF EQUILIBRIUM COMPOSITIONS**

by

**Chen C. Hsu, Robert H. Land,
and M. Blander**

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Chemical Engineering Division

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ABSTRACT

A NASA computer program for calculation of complex equilibrium compositions has been modified to take into account the formation of an ideal binary solution from pure condensed species. The thermodynamics of the modification are discussed. Applications are presented.

I. INTRODUCTION

For a simple chemical reaction, the equilibrium compositions can be calculated through the equilibrium constant approach (mass action law). However, when complex chemical reactions are involved, there are too many reaction equations to be solved even approximately. For instance, the combustion of a hydrocarbon in air may involve some twenty or more chemical reactions. In the combustion of coal for conventional and MHD (magneto-hydrodynamics) power generation and in the formation of meteorites, the reactions become even more complicated. The only possible way for obtaining the solutions of a number of simultaneous equations is by the use of trial and error as an iterative method. The first major advance in the iterative approach was due to S. R. Brinkley^{1,2} who paved the way for a systematic scheme for equilibrium computation. Briefly, Brinkley's method is first to select a number of components and through the use of chemical equilibrium constants, to compute the concentrations of every possible species in the equilibrium mixture. The species concentrations obtained are in turn used as corrections to the atom balance equations, and the correction procedure involves solving a set of corrected equations by using the Newton-Raphson linearization method.³ The problem associated with this method is that its success is very much dependent on the user's intuition to predict the possible products of the reaction. Needless to say, the computer code has to be modified once the chemical system is changed. As a result, this method is regarded as being rather tedious and cumbersome. The other method for solving chemical equilibrium compositions is by minimization of the system free energy. This method was developed by White, Johnson and Dantzig.⁴ They defined the equilibrium constants in terms of free energy and included the rigorous phase equilibrium relationships in the calculation. A detailed review paper by Zeleznik and Gordon⁵ has an excellent account of these two different approaches.

Gordon and McBride developed a so-called NASA CEC code,⁶ based on the minimization of the free energy of a system, in order to obtain the equilibrium composition of a complex chemical system. Throughout the calculation, ideal gases and pure condensed species are assumed. The selection of the possible stable species is made by accessing a chemical data base containing

chemical formulas and their coefficients of thermodynamic functions, C_p , S and ΔH , which were evaluated essentially from the JANAF Thermochemical Tables.⁷ The computer program has four functions: (1) to calculate chemical equilibrium for an assigned thermodynamic state defined by the following combinations of two variables:

- (a) temperature and pressure (TP)
- (b) enthalpy and pressure (HP)
- (c) entropy and pressure (SP)
- (d) temperature and volume or density (TV)
- (e) internal energy and volume or density (UV)
- (f) entropy and volume or density (SV);

(2) to evaluate theoretical performance for both equilibrium and frozen compositions during expansion; (3) to calculate incident and reflected shock properties; and (4) to calculate Chapman-Jonquet detonation properties. In all these, the pure condensed species are taken into account. Besides its multiple purposes, the simplicity and versatility of the computer program led to wide use. Practically, one could easily obtain the equilibrium compositions of a chemical system by inputting the thermodynamic information of the reactants. The NASA CEC code does, however, leave room for improvement, namely, taking into account the possibility of formation of both ideal and nonideal solution phases. The first phase of the improvement, which includes the possibility of the formation of ideal binary solutions, has been carried out. The thermodynamic principles of the ideal binary solution, the details of the modifications of the computer code, and the successful tests will be described in this report.

II. THERMODYNAMIC PRINCIPLES

It is assumed that it is possible to form a solution of two components from a mixture of ideal gaseous species. The system Gibbs free energy, g , is expressed as:

$$g = \sum_{j=1}^n \mu_j n_j + g_{sol} \quad (1)$$

where $g_{sol} = n_\alpha \mu_\alpha + n_\beta \mu_\beta$, the Gibbs free energy of the solution and n = the total number of gaseous and pure condensed species. The μ_j , n_j are the chemical potentials and number of moles of the j th species in the gaseous or pure condensed species, while μ_α , n_α , and μ_β and n_β are the chemical potentials and number of moles of α , β components of the solution, respectively. We have assumed ideality of the solutions in the calculation; thus the chemical potentials of the gaseous species, the pure condensed species, and the components of the solution can be expressed as:

$$\mu_j = \mu_j^\circ + RT \ln \left(\frac{n_j}{n} \right) + RT \ln p \quad (2)$$

for pure condensed species,

$$\mu_j = \mu_j^\circ \quad (3)$$

and for component α of the solution,

$$\mu_\alpha = \mu_\alpha^\circ + C_\alpha RT \ln \frac{C_\alpha n_\alpha}{C_\alpha n_\alpha + C_\beta n_\beta} \quad (4)$$

where μ_α° denotes the chemical potential in the standard state, and C_α , C_β are the stoichiometric coefficients of the cations of the α and β components, respectively. For the ideal case, C_α and C_β are set to equal to 1. One may write g_{sol} explicitly as

$$\begin{aligned} g_{\text{sol}} &= n_\alpha \mu_\alpha + n_\beta \mu_\beta = n_\alpha (\mu_\alpha^\circ + C_\alpha RT \ln \frac{C_\alpha n_\alpha}{C_\alpha n_\alpha + C_\beta n_\beta}) \\ &\quad + n_\beta (\mu_\beta^\circ + C_\beta RT \ln \frac{C_\beta n_\beta}{C_\alpha n_\alpha + C_\beta n_\beta}) \end{aligned} \quad (5)$$

The condition for chemical equilibrium is the minimization of free energy. The minimization is subject to certain constraints such as the following mass balance constraint:

$$\sum_{j=1}^n a_{ij} n_j - b_i^\circ = 0 \quad i = 1, \dots, l \quad (6)$$

where a_{ij} , b_i° are the number of moles of element i per mole of species j , and the assigned number of moles of element i per kilogram of total reactants, respectively, and l = the total number of elements in the system. If one defines a term G to be

$$G = g + \sum_{i=1}^n \lambda_i (b_i - b_i^\circ) \quad (7)$$

where λ_i are Lagrangian multipliers, the condition for equilibrium becomes

$$\begin{aligned} \delta G &= \sum_{j=1}^n (\mu_j + \sum_{i=1}^l \lambda_i a_{ij}) \delta n_j + \left[\left(\frac{\partial g_{\text{sol}}}{\partial n_\alpha} \right) + \sum_{i=1}^l \lambda_i a_{i\alpha} \right] \delta n_\alpha \\ &\quad + \left[\left(\frac{\partial g_{\text{sol}}}{\partial n_\beta} \right) + \sum_{i=1}^l \lambda_i a_{i\beta} \right] \delta n_\beta + \sum_{i=1}^l (b_i - b_i^\circ) \delta \lambda_i = 0 \end{aligned} \quad (8)$$

$$\text{where } b_i = \sum_{j=1}^n a_{ij} n_j$$

If one treats δn_j , δn_α , δn_β , and $\delta \lambda_i$ as independent variables, one obtains

$$\mu_j + \sum_{i=1}^l \lambda_i a_{ij} = 0 \quad j = 1, \dots, n \quad (9)$$

$$\left(\frac{\partial g_{sol}}{\partial n_\alpha} \right) + \sum_{i=1}^l \lambda_i a_{i\alpha} = 0 \quad (10)$$

$$\left(\frac{\partial g_{sol}}{\partial n_\beta} \right) = \sum_{i=1}^l \lambda_i a_{i\beta} = 0, \text{ and} \quad (11)$$

$$b_i - b_i^\circ = 0 \quad (12)$$

where

$$\left(\frac{\partial g_{sol}}{\partial n_\alpha} \right) = n_\alpha \left(\frac{\partial \mu_\alpha}{\partial n_\alpha} \right) + \mu_\alpha + n_\beta \left(\frac{\partial \mu_\beta}{\partial n_\alpha} \right) \quad (13)$$

$$\left(\frac{\partial g_{sol}}{\partial n_\beta} \right) = n_\beta \left(\frac{\partial \mu_\beta}{\partial n_\beta} \right) + \mu_\beta + n_\alpha \left(\frac{\partial \mu_\alpha}{\partial n_\beta} \right) \quad (14)$$

By the Gibbs-Duhem relation, one can rewrite Eqs. 10 and 11

$$\mu_\alpha + \sum_{i=1}^l \lambda_i a_{i\alpha} = 0 \quad (15)$$

$$\mu_\beta + \sum_{i=1}^l \lambda_i a_{i\beta} = 0 \quad (16)$$

The descent Newton-Raphson method³ is used to solve for corrections to initial estimates of n_j , λ_i , n , n_α , n_β , and T if required. As we are interested in solving for n_α and n_β , Gibbs iteration equations are obtained by using a Taylor series expansion only to the first derivative.

$$-\sum_{i=1}^l \pi_i a_{i\alpha} + \frac{C_\alpha C_\beta n_\beta}{n_\alpha (C_\alpha n_\alpha + C_\beta n_\beta)} \Delta n_\alpha - \frac{C_\alpha C_\beta}{(C_\alpha n_\alpha + C_\beta n_\beta)} \Delta n_\beta = -\frac{\mu_\alpha}{RT} \quad (17)$$

$$-\sum_{i=1}^l \pi_i a_{i\beta} - \frac{C_\alpha C_\beta}{(C_\alpha n_\alpha + C_\beta n_\beta)} \Delta n_\alpha + \frac{C_\alpha C_\beta n_\alpha}{n_\beta (C_\alpha n_\alpha + C_\beta n_\beta)} \Delta n_\beta = -\frac{\mu_\beta}{RT} \quad (18)$$

where $\pi_i = -\lambda_i / RT$.

The coefficients of vectors of Δn_α and Δn_β in Eqs. 17 and 18 become four elements of the matrix, in addition to the elements that already exist for gaseous and pure condensed species. This portion of the derivation has been implemented and successfully tested.⁸ The Helmholtz free energy, which is a function of temperature and volume, was not used in this modification of the computer codes.

III. MODIFICATIONS OF COMPUTER CODES

We are interested only in the computation of equilibrium compositions. Thus, the following nonrelevant subroutines were deleted from the NASA CEC code: Subroutine ROCKET, Subroutine RKTOUT, Subroutine FROZEN, Subroutine SHK, and Subroutine DETON.

The main modification of the NASA CEC code is the inclusion of an option to seek the formation of a binary solution after the completion of the regular program functions, *i.e.*, the selection of stabilized gas and pure condensed species. In order to let the system look for the possibility of forming a binary solution, the solution components and the initial estimates of their concentrations have to be assigned. With the addition of two more species, the dimension of the matrix is increased by two, Eqs. 17 and 18. The dimensions of the variables involved in the matrix therefore have to be increased accordingly. The main program, along with the following four subroutines are involved: Subroutine SEARCH, Subroutine EQLBRM, Subroutine MATRIX, and Subroutine THERMP (Fig. 2). The details of the modifications are described as follows:

Main Program

The main program flow is illustrated in Fig. 1. The main modifications are:

- (1) the double precision variables EN10, EN20, C1, C2, for the initial estimates of concentrations, and stoichiometric ratios of cations for components 1 and 2, respectively, are defined, and put in a labeled COMMON block, (see Appendix A for definition of common variables);
- (2) the variables SOLU, SOLN, COMP are defined in integer variables;
- (3) the variables in COMMON block, SOLN (6,3) for the chemical formulas of solution components, NSOLN for the number of components; IS as a flag for solution; JSOL1, JSOL2 for the indices of the concentration of solution components are defined;
- (4) the variables SOLU and COMP are defined in a DATA statement;
- (5) two code cards are added, one with SOLUTION, the other with COMPOUND;
- (6) chemical formulas are stored in SOLN (6,3) after code card SOLUTION has been read;
- (7) the initial concentrations EN10, EN20, and stoichiometric ratios C₁, C₂ are read after code card COMPOUND has been read;
- (8) the initial estimates of concentrations and the stoichiometric ratios are printed out; and
- (9) IS is set = 0.

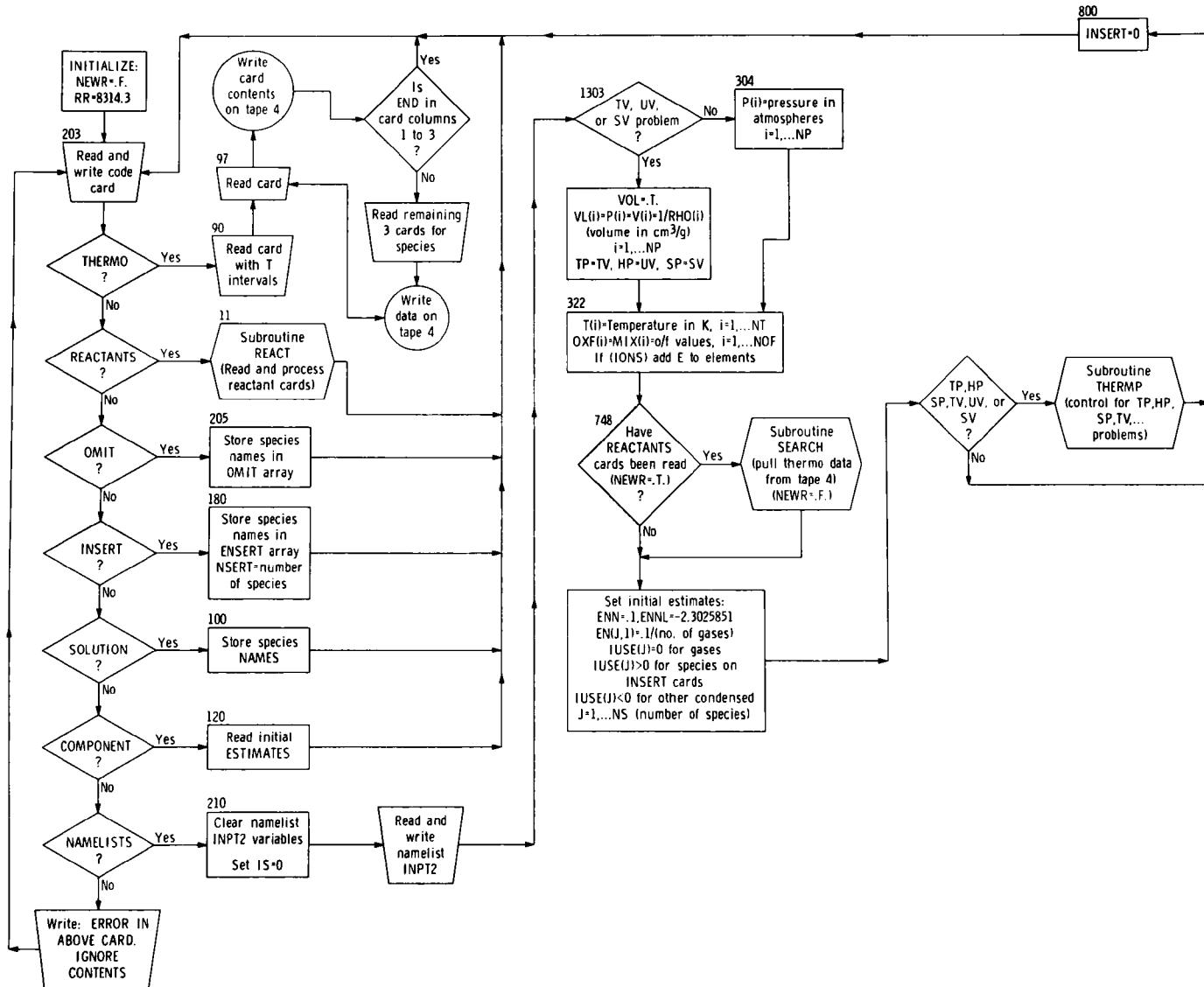


Fig. 1. Flow Diagram for Main Routine.

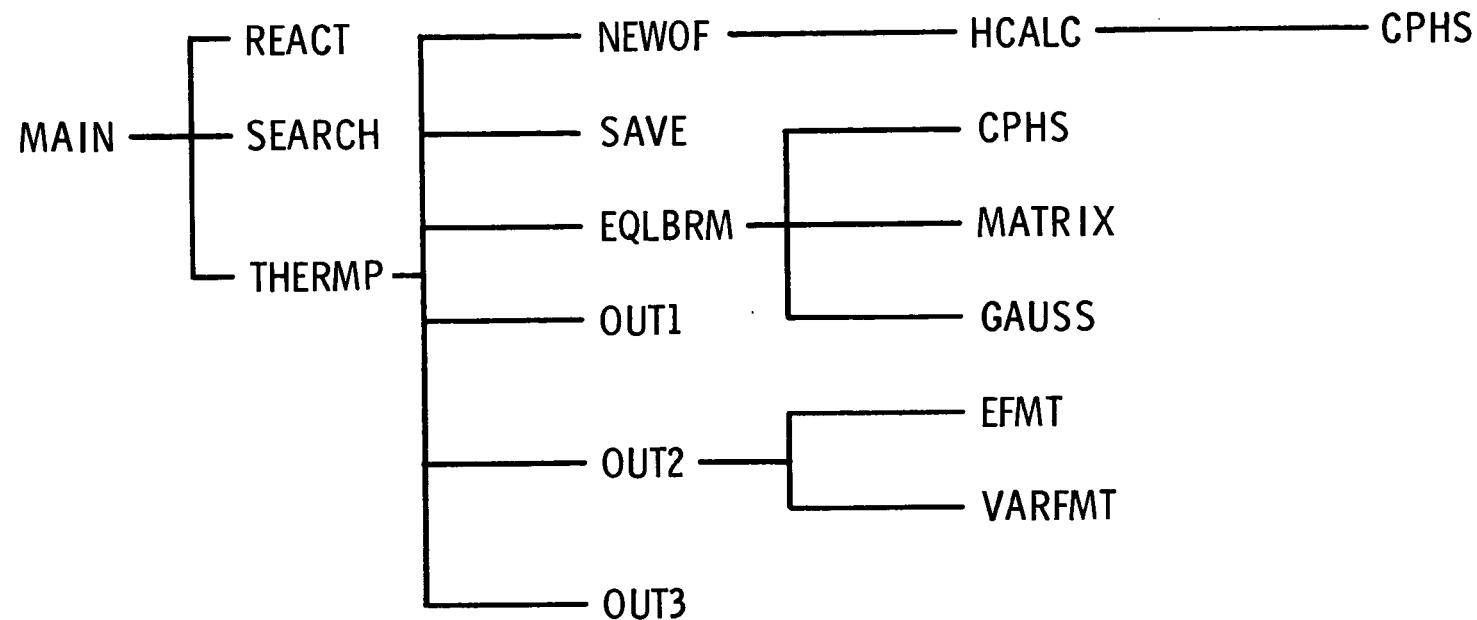


Fig. 2. Subroutine Tree Diagram.

Subroutine SEARCH

In this subroutine, thermodynamic data from the chemical data base are read, and the data of the matched species are stored. The modification is in the area of matching these solution components. The modifications are as follows:

- (1) the matched species from the data base with the assigned solution components are labeled with -999 as the value of the proper elements of the IUSE array;
- (2) a logic IF is set up to check the species labeled with the element of ISUE = -999 in the selection of the condensed species;
- (3) the total number of condensed species, NS, is increased by one, once label -999 is detected; and
- (4) the selected components for the solution phase are printed.

Subroutine EQLBRM

This subroutine calculates equilibrium compositions and thermodynamic properties for a particular set of input data. The flow chart of the modified subroutine is shown in Figs. 3 and 4. The modifications to incorporate the existing code are:

- (1) the concentrations of solution components are changed to 10^{-12} if they become negative in the iteration process;
- (2) the concentration distributions for species greater than 10^{-50} are printed when the subroutine does not converge after a certain number of iterations;
- (3) the value of the flag IS is set to 1 at the point when the computer looks into the possibility of solution formation after the selection of gas and pure condensed species. The logical variable CONVG is set equal to False before additional iterations begin;
- (4) the index IQ1, which is the number of elements plus the number of condensed species plus 1, is increased by 2;
- (5) the initial estimates of concentrations are assigned to the proper solution components which carry IUSE value -999 and which are in the temperature range of interest;
- (6) the IUSE value is changed to 999 for solution components after the initial estimates of concentrations have been assigned; and
- (7) the subroutine CPHS for the calculation of thermodynamic properties is called, and the program flow is directed to repeat the iteration process.

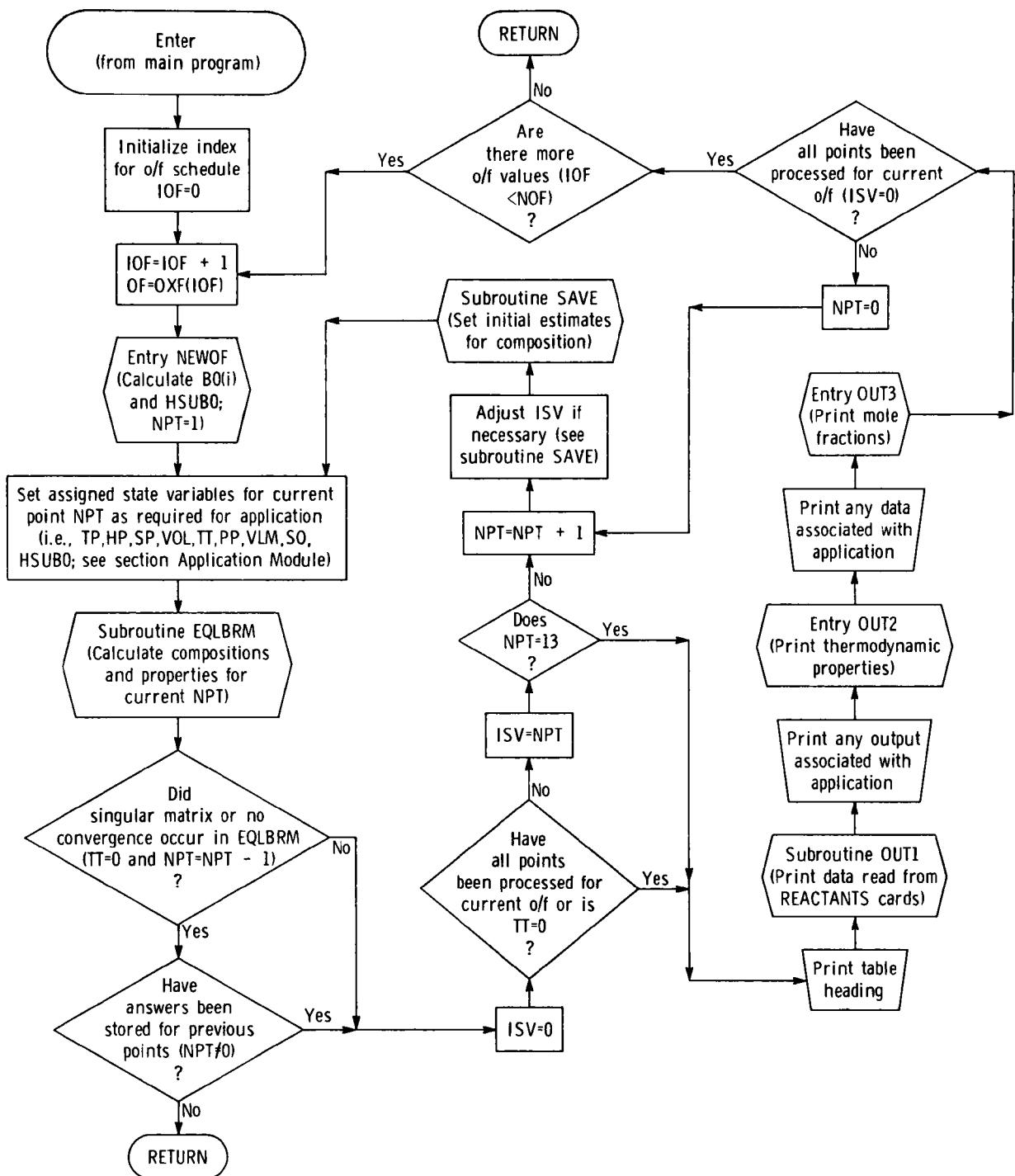


Fig. 3. Flow Diagram of an Application Module.

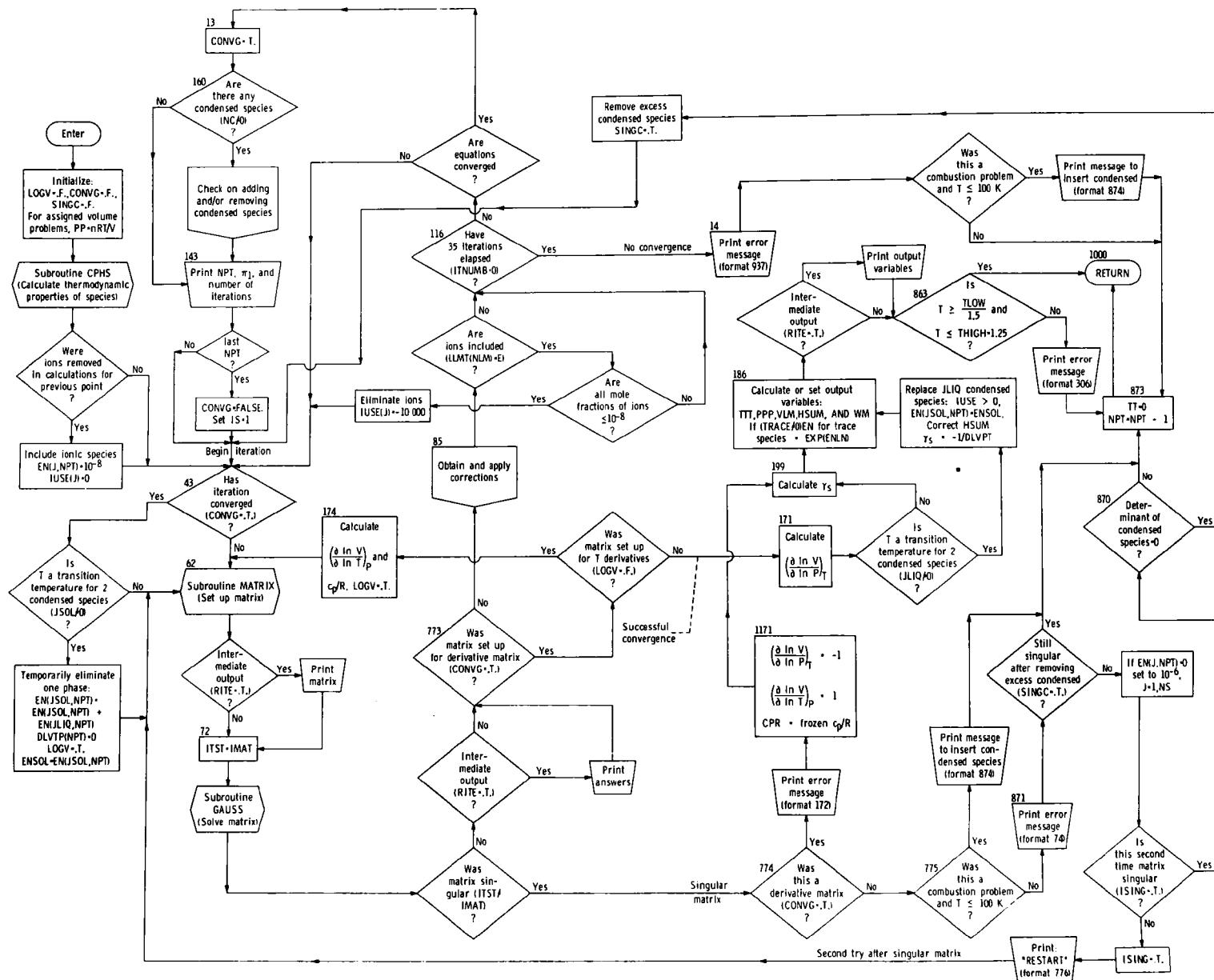


Fig. 4. Flow Diagram for Subroutine EQLBRM

Subroutine MATRIX

This subroutine sets up matrices according to the assigned conditions. In this modification it is the assigned temperature and pressure. The main part of the inclusion of the modified matrix is based on Eq. 17 and 18. The dimension of the matrix is increased by two - (two rows and two columns), Table 1. The modifications are as follows:

(1) the species with the value of IUSE equal to 999 at the beginning of setting up the iteration matrix are selected;

(2) if IS = 0, the subroutine skips the evaluation of solution components. If IS = 1, the subroutine sets the indices of the matrix for the solution components; and

(3) if IS = 1, the elements of the augmented matrix are calculated using Eqs. 17 and 18.

Subroutine THERMP

In this subroutine the common variables are set according to the assigned thermodynamic states, *i.e.*, temperature and pressure. Before calling subroutine EQLBRM, the following modifications were made:

(1) the species considered by the system are checked for a negative value of concentration. If there is a negative value, then IS is reset to zero. The indices of the matrix are readjusted and the value of IUSE is set so that it starts fresh for the calculation of the next assigned thermodynamic state. If there is no negative value, the subroutine continues the regular program flow;

(2) the concentrations, the values of the natural logarithm of the concentrations of the species considered by the system are initialized. For the condensed species, the initial concentration is set equal to zero, whereas for gas species, the concentration is set equal to 0.1.

(3) continues the regular program flow after (2) has been carried out.

The information described above gave the details of the modifications for the computer program. For details of the computer program, the source program is attached as Appendix B.

IV. PROGRAM INPUT AND OUTPUT

In addition to the input information required by the original NASA CEC code⁶ such as (a) REACTANTS code card, (b) REACTANTS cards, (c) OMIT and/or INSERT cards, if any, (d) NAMELISTS code card, and (e) NAMELISTS data, the modified code requires the following additional cards:

- (a) SOLUTION code card,
- (b) SOLUTION data,
- (c) COMPOUND code card,
- (d) COMPOUND data.

Table 1. Iteration Equations to Determine Equilibrium Compositions for Assigned Temperature and Pressure.

Variables											
Equation	π_1	π_2	---	π_ℓ	Δn_{m+1}	---	Δn_n	Δn_α	Δn_β	$\Delta \ln n$	Right side
†	$\sum_{j=1}^m a_{1j} a_{1j} n_j$	$\sum_{j=1}^m a_{1j} a_{2j} n_j$	---	$\sum_{j=1}^m a_{1j} a_{\ell j} n_j$	$a_{1,m+1}$	---	a_{1n}	$a_{1\alpha}$	$a_{1\beta}$	$\sum_{j=1}^m a_{1j} n_j$	$(b_1^0 - b_1) + \sum_{j=1}^m a_{1j} n_j G_j$
	$\sum_{j=1}^m a_{2j} a_{1j} n_j$	$\sum_{j=1}^m a_{2j} a_{2j} n_j$	---	$\sum_{j=1}^m a_{2j} a_{\ell j} n_j$	$a_{2,m+1}$	---	a_{2n}	$a_{2\alpha}$	$a_{2\beta}$	$\sum_{j=1}^m a_{2j} n_j$	$(b_2^0 - b_2) + \sum_{j=1}^m a_{2j} n_j G_j$
††	$\sum_{j=1}^m a_{\ell j} a_{1j} n_j$	$\sum_{j=1}^m a_{\ell j} a_{2j} n_j$	---	$\sum_{j=1}^m a_{\ell j} a_{\ell j} n_j$	$a_{\ell,m+1}$	---	$a_{\ell n}$	$a_{\ell\alpha}$	$a_{\ell\beta}$	$\sum_{j=1}^m a_{\ell j} n_j$	$(b_\ell^0 - b_\ell) + \sum_{j=1}^m a_{\ell j} n_j G_j$
	$a_{1,m+1}$	$a_{2,m+1}$	---	$a_{\ell,m+1}$	0	---	0	0	0	0	G_{m+1}
(17)	a_{1n}	a_{2n}	---	$a_{\ell n}$	0	---	0	0	0	0	G_n
	$a_{1\alpha}$	$a_{2\alpha}$	---	$a_{\ell\alpha}$	0	---	0	$-\frac{C_\alpha C_\beta n_\beta}{n_\alpha \text{SUMI}}$	$\frac{C_\alpha C_\beta}{\text{SUMI}}$	0	G_α^{**}
(18)	$a_{1\beta}$	$a_{2\beta}$	---	$a_{\ell\beta}$	0	---	0	$\frac{C_\alpha C_\beta}{\text{SUMI}*}$	$\frac{C_\alpha C_\beta n_\beta}{n_\beta \text{SUMI}}$	0	G_β
***	$\sum_{j=1}^m a_{1j} n_j$	$\sum_{j=1}^m a_{2j} n_j$	---	$\sum_{j=1}^m a_{\ell j} n_j$	0	---	0	0	0	$\sum_{j=1}^m n_j - n$	$n - \sum_{j=1}^m n_j + \sum_{j=1}^m n_j G_j$

*SUMI = $1/(C_\alpha n_\alpha + C_\beta n_\beta)$, **G = μ/RT , *** $\sum_{i=1}^\ell \sum_{j=1}^m a_{ij} n_j \pi_i + (\sum_{j=1}^m n_j - n) \Delta \ln n = n - \sum_{j=1}^m n_j + \sum_{j=1}^m n_j G_j$ for gas species.

+ $\sum_{i=1}^\ell \sum_{j=1}^m a_{kj} a_{ij} n_j \pi_i + \sum_{j=m+1}^n a_{kj} \Delta n_j + \sum_{j=1}^m a_{kj} n_j \Delta \ln n = (b_k^0 - b_k) + \sum_{j=1}^m a_{kj} n_j G_j$ ($k=1, \dots, \ell$) for gas species.

†† $\sum_{i=1}^\ell a_{ij} \pi_i = G_j$ ($j=m+1, \dots, n$) for pure condensed species.

The SOLUTION data card which uses the same SOLUTION code card gives the chemical formulas of the assigned solution components, whereas the COMPOUND data card uses a separate card for initial concentration estimates of the species (in kg-mol/kg mixture) and the stoichiometric ratios of cations. The contents of the program input and the formats of SOLUTION and COMPOUND code cards are shown in Tables 2 and 3, respectively.

As the regular program functions, the information on input cards are output once they are read. With the addition of SOLUTION and COMPOUND cards, they are printed out as parts of the computer output. In addition, the initial estimates of the species concentrations as well as the stoichiometric ratios of cations are printed. A special message with the heading of "Selected Components for Solution Phase Are:" is listed to enable the user to check the exact solution components being considered. The rest of the program output remains unchanged. For a sample program input and output, one may refer to Appendix D for detail.

V. THERMODYNAMIC DATA

Thermodynamic data are essentially taken from JANAF Tables,⁷ with some from Robie and Waldbaum.⁹ Some 66 species have been added to the data base since 1976 making a total of 737 species. The thermochemical information for each individual species is Cp, ΔH and S. A separate program-PAC¹⁰ was used to fit simultaneously fourteen coefficients of the following functional forms in two temperature ranges 300-1000 K and 1000-5000 K:

$$\frac{C_p}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4 \quad (19)$$

$$\frac{H_T}{RT} = a_1 + \frac{a_2}{2} T + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T} \quad (20)$$

$$\frac{S_T}{R} = a_1 \ln T + a_2 T + \frac{a_3}{2} T^2 + \frac{a_4}{3} + \frac{a_5}{4} T^4 + a_7 \quad (21)$$

The coefficients so obtained are used as the input for the data base. The updated listing of the data base is given in Appendix C.

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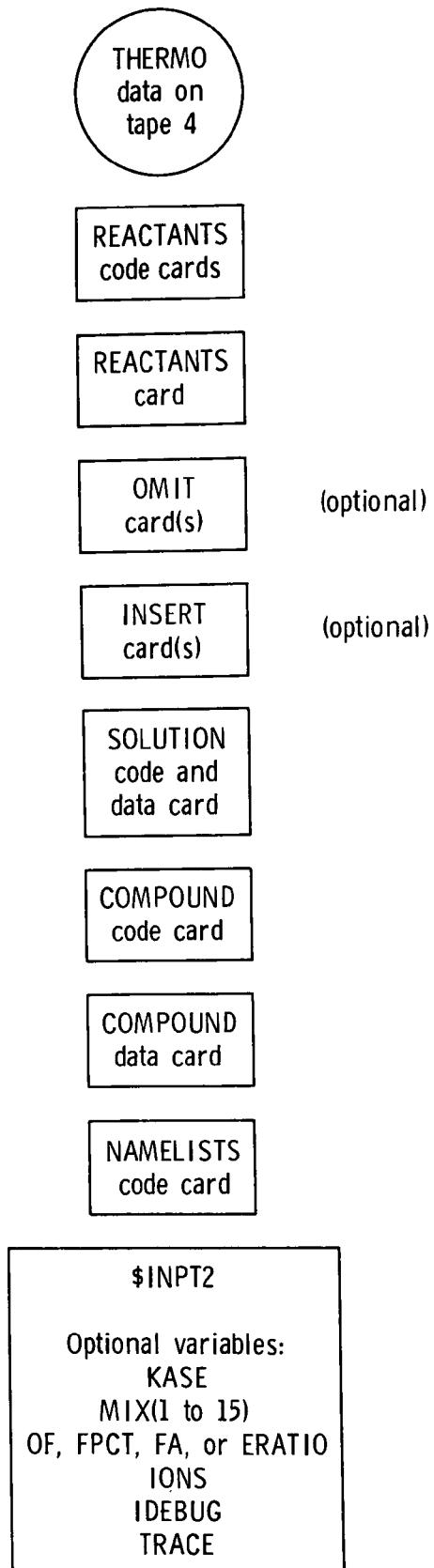


Table 2. Program Input.

Table 3. Solution and Compounds Cards

Order	Contents	Format
Between REACTANTS and NAMELISTS cards	SOLUTION	5(3A4, 3X)
Following SOLUTION code cards	COMPOUND	3A4
Following COMPOUND code cards	One card for the initial concentrations and the cations stoichiometric ratios of the binary solution components	2D15.7, 2F5.0

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APPENDICES

Appendix A

COMMON VARIABLES

The variables used in the modification are defined and described in this appendix. For variables used in the original NASA CEC code, Ref. 6 should be consulted.

<u>Variables</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
C1		COMP	Main EQLBRM MATRIX	The stoichiometric ratio of the cation of the first solution component.
C2		COMP	Main EQLBRM MATRIX	The stoichiometric ratio of the cation of the second solution component.
EN1			MARTIX	The concentration of the first solution component in kg-mol/kg of mixture.
EN2			MARTIX	The concentration of the second solution component in kg-mol/kg of mixture.
EN10		COMP	Main EQLBRM MATRIX	The initial estimate of the concentration of the first solution component in kg-mol/kg mixture.
EN20		COMP	Main EQLBRM MARTIX	The initial estimate of the concentration of the second solution component in kg-mol/kg mixture.
IS		IS	Main EQLBRM MARTIX THERMP	A flag to indicate whether the system has considered solution information. When IS = 0, the solution is not considered; when IS = 1, the solution is being considered.
IUSE	250	SPECES	Main EQLBRM CPHS MATRIX HCALC SAVE SEARCH	The original variables of the NASA CEC code. But additional value of IUSE, 999, has been assigned to represent the solution components.

Appendix A (Cont'd)

<u>Variables</u>	<u>Dimension</u>	<u>Common Label</u>	<u>Routines Where Used</u>	<u>Description and Comments</u>
JSOL1		IS	Main EQLBRM MATRIX THERMP	The index of the matrix for the first solution component.
JSOL2		IS	Main EQLBRM MATRIX THERMP	The index of the matrix for the second solution component.
KK1		MATRIX		KK1 = KK+1 where KK is the total number of reactant elements. KK1 is used as the index of the solution of the matrix for the first solution component.
KK2		MATRIX		KK2 = KK+2 where KK is the total number of reactant elements. KK2 is used as the index of the solution of the matrix for the second solution component.
NSOLN		SOLN	Main SEARCH	The number of the solution components. In this binary solution model, NSOLN = 2.
RAT1		MATRIX		RAT1 = C1 x EN1 x SUMI, a part of Eq. 17.
RAT2		MATRIX		RAT2 = C2 x EN2 x SUMI, a part of Eq. 18.
SOLN	6,3	SOLN	Main SEARCH	The chemical formulas of the solution components.
SUMI			MATRIX	SUMI = $\frac{1.0}{C1 \times EN1 + C2 \times EN2}$, common factor of Eqs. 17 and 18.

Appendix B
PROGRAM LISTING

C	MAIN PROGRAM	MAIN	1
	DCUBLE PRECISION G,X	MAIN	3
	DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS	MAIN	8
	DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN	MAIN	9
	DOUBLE PRECISION EN10,EN20,C1,C2	SOLN	
C	REAL MIX(15)	MAIN	10
	INTEGER DATA, OMIT, ENSERT, REAC, BLANK, THRM, END, SUB	MAIN	11
	INTEGER SOLU,SOLN,COMP	SOLN	
	LOGICAL SHOCK,MMHG,UV,IC,DETN,SIUNIT,EUNITS,NSQM,CALCH	MAIN	13
	LOGICAL HF,SP,TP,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV,SV	MAIN	14
	LOGICAL FA,OF,ERATIO,FPCT,OTTO	MAIN	15
C	DIMENSION OMIT(3,3),NCD(4),ENSLERT(3,3),RHO(26),LVP(2),VM(2),VL(26)	MAIN	17
	1,DAT(22)	MAIN	18
	CCMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)	MAIN	19
	1,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)	MAIN	20
	2,VLM(13),TOTN(13)	MAIN	21
	COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250)	MAIN	22
	1,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250)	MAIN	23
	COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)	MAIN	24
	1,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	MAIN	25
	2,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)	MAIN	26
	3,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)	MAIN	27
	4,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE,SIZE	MAIN	28
	COMMON /DOUBLE/ G(20,21), X(20)	MAIN	29
	COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES, NP, NT, NPT, NLM	MAIN	30
	1, NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ	MAIN	31
	2, IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH	MAIN	32
	3,IQSAVE,LSAVE,ISUP,ISUB,ITNUM	MAIN	33
	COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13)	MAIN	34
	1,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT	MAIN	35
	COMMON/SOLN/SOLN(6,3),NSOLN	SOLN	
	CCMMCN/COMP/EN10,EN20,C1,C2	SOLN	
C	COMMON/IS/IS,JSOL1,JSOL2	SOLN	
C	EQUIVALENCE (OMIT,ENLN),(ENSLERT,DELN),(OXF,MIX)	MAIN	36
	1,(OF,OXFL),(RHO,P,VI),(S0,SO),(OTTO,CPCVFR),(DATA,DAT)	MAIN	37
	DATA MIT/4HOMIT/,BLANK/1H/, PSIA/4HPSIA/, REAC/4HREAC/,IZ/2H00/	MAIN	38
	1,NMLT/4H NAME/,IE/1HE/,INSERT/4HINSE/,THRM/4HTHER/,END/3HEND/	MAIN	40
	2,GAS/1HG/,LAST/4HLAST/	MAIN	41
C	DATA SOLU/4HSOLU/,COMP/4HCOMP/	MAIN	42
	NAMELIST/INPT2/KASE,T,P,PSIA,MMHG,NSQM,V,RHO,ERATIO,OF,FPCT,FA,	SOLN	
	1MIX,TP,HP,SP,TV,UV,SV,RKT,SHOCK,DETN,OTTO,CR,S0,SO,IONS,IDEBUG,	MAIN	44
	2TRACE,SIUNIT,EUNITS	MAIN	45
C	NEWR = .FALSE.	MAIN	46
C	1 WRITE(6,400)	MAIN	47
	400 FORMAT(1H1)	MAIN	48
	RR = 8314.3	MAIN	49
	NOMIT = 0	MAIN	50
	NSOLN = 0	MAIN	51
	R = RR/4184.	SOLN	
	203 READ(5,204,END=2001) (DATA(I),I=1,15)	SOLN	
	204 FORMAT(5(3A4,3X))	MAIN	53
	WRITE (6,2045)(DATA(I),I=1,15)	MAIN	55
		MAIN	56

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2045 FORMAT(1X,5(3A4,3X))          MAIN  57
  IF(DATA(1).EQ.THRM) GO TO 90    MAIN  58
  IF(DATA(1).EQ.REAC) GO TO 11    MAIN  59
  IF (DATA(1).EQ.MIT) GO TO 205   MAIN  60
  IF (DATA(1).EQ.INSERT) GO TO 180  MAIN  61
  IF(DATA(1).EQ.NMLT) GO TO 210   MAIN  62
  IF(DATA(1).EQ.BLANK) GO TO 203   MAIN  63
  IF(DATA(1).EQ.SOLU) GO TO 100    SOLN
  IF(DATA(1).EQ.COMP) GO TO 120    SOLN
1023 WRITE(6,1024)                 MAIN  64
1024 FORMAT(40HOERROR IN ABOVE CARD. CONTENTS IGNORED. )  MAIN  65
  GO TO 203                      MAIN  66
11  NSERT = 0                      MAIN  67
  MOLES = .FALSE.                  MAIN  68
  CALL REACT                      MAIN  69
  IF(NLM.EQ.0) WRITE(6,52)          MAIN  70
52  FCRMAT(24HOERROR IN REACTANT CARDS)  MAIN  71
  CALCH = .FALSE.                  MAIN  72
  DO 755 N=1,NREAC                MAIN  73
  IF(NAME(N,5).EQ.IZ) CALCH=.TRUE.  MAIN  74
755 CONTINUE                      MAIN  75
  GO TO 203                      MAIN  76
C
C      READ THERMO DATA FROM CARDS AND STORE ON TAPE 4  MAIN  77
C
90  NEWR = .TRUE.                  MAIN  78
  REWIND 4                        MAIN  79
  READ(5,5) TLLOW,TMID,THIGH       MAIN  80
  5 FORMAT (3F10.3)                MAIN  81
  WRITE (4,5) TLLOW,TMID,THIGH     MAIN  82
97  READ (5,10) (DAT(I),I=1,16),NCD(1)  MAIN  83
10  FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3,I15)  MAIN  84
  IF(DATA(1).EQ.BLANK) DATA(1)=END  MAIN  85
  WRITE (4,10) (DAT(I),I=1,16)      MAIN  86
  IF(DATA(1).NE.END) GO TO 18      MAIN  87
  WRITE(4,10) LAST                 MAIN  88
  GO TO 203                      MAIN  89
18  READ(5,20) (DAT(I),I=1,5),NCD(2),(DAT(J),J=6,10),NCD(3),(DAT(K),
  1K=11,14),NCD(4)               MAIN  90
20  FORMAT(5E15.8,I5/5E15.8,I5/4E15.8,I20)  MAIN  91
  WRITE (4,21) (DAT(I),I=1,14)      MAIN  92
21  FORMAT(5E15.8/5E15.8/4E15.8)    MAIN  93
  DO 25 I=1,4                     MAIN  94
  IF(NCD(I).EQ.I) GO TO 25        MAIN  95
  WRITE(6,22) (DATA(J),J=1,3)      MAIN  96
22  FORMAT(28HOERROR IN ORDER OF CARDS FOR ,3A4)  MAIN  97
25  CONTINUE                      MAIN  98
  GO TO 97                        MAIN  99
C
C      CHECK INSERT CARDS          MAIN 100
C
180 DO 185 I=4,15,3              MAIN 101
  IF (DATA(I).EQ.BLANK) GO TO 185  MAIN 102
  NSERT = NSERT+1                 MAIN 103
  ENSERT(1,NSERT) = DATA(I)        MAIN 104
  ENSERT(2,NSERT) = DATA(I+1)      MAIN 105
  ENSERT(3,NSERT) = DATA(I+2)      MAIN 106
185 CONTINUE                      MAIN 107
  GO TO 203                      MAIN 108
                                         MAIN 109
                                         MAIN 110
                                         MAIN 111
                                         MAIN 112
                                         MAIN 113

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C          CHECK OMIT CARDS
C
205 DO 208 I=4,15,3           MAIN 114
  IF(DATA(I).EQ.BLANK) GO TO 208
  NCMIT = NOMIT+1             MAIN 115
  OMIT(1,NOMIT) = DATA(I)     MAIN 116
  OMIT(2,NOMIT) = DATA(I+1)   MAIN 117
  OMIT(3,NOMIT) = DATA(I+2)   MAIN 118
208 CONTINUE                  MAIN 119
  NEWR=.TRUE.
  REWIND 4                     MAIN 120
  GO TO 203                   MAIN 121
100 DC 110 I=4,15,3           MAIN 122
  IF(DATA(I).EQ.BLANK) GO TO 110
  NSOLN = NSOLN+1              MAIN 123
  IF(NSOLN.GT.2) GO TO 203    MAIN 124
  SCLN(1,NSOLN) = DATA(I)     MAIN 125
  SCLN(2,NSOLN) = DATA(I+1)   MAIN 126
  SCLN(3,NSOLN) = DATA(I+2)
110 CONTINUE                  SOLN
  GO TO 203                   SOLN
120 READ2000,EN10,EN20,C1,C2
2000 FFORMAT(2D15.7,2D5.0)      SOLN
125 PRINT 3000,EN10,EN20,C1,C2
3000 FORMAT(' N1=',1PD15.7,5X,'N2=',1PD15.7,5X,'C1=',0PD8.1,
15X,'C2=',D8.1)
  GO TO 203                   SOLN
C
C          BEGIN NAMELIST INPT2
C
210 DC 300 I=1,26             MAIN 127
  P(I)=0.
  T(I)=0.
  V(I)=0.
300 CONTINUE                  MAIN 128
  IS=0
  TRACE=0.
  SC=0.
  V1=0.
  V2=0.
  CR=0.
  RHOP=0.
  KASE=0
  TP=.FALSE.
  HP=.FALSE.
  SP=.FALSE.
  TV=.FALSE.
  UV=.FALSE.
  SV=.FALSE.
  OTTO=.FALSE.
  RKT=.FALSE.
  SHOCK=.FALSE.
  DETN=.FALSE.
  VOL=.FALSE.
  MMHG=.FALSE.
  PSIA=.FALSE.
  NSQM=.FALSE.
  SIUNIT=.FALSE.

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EUNITS = .FALSE.
IONS = .FALSE.
IDEBUG = 0
FA= .FALSE.
OF= .FALSE.
ERATIO = .FALSE.
FPCT= .FALSE.
DO 303 I=1,15
MIX(I) = 0.
303 CONTINUE
NT = 1
EQL = .TRUE.
READ(5,INPT2)
WRITE(6,INPT2)
IF(.NOT.DETN.AND..NOT.SHOCK) GO TO 1303
DO 1300 N=1,NREAC
IF(FAZ(N).NE.GAS) GO TO 1301
1300 CONTINUE
GO TO 1303
1301 WRITE(6,1302)
1302 FORMAT(60H0CONDENSED REACTANTS NOT PERMITTED IN DETN OR SHOCK PROB
1LEMS)
GO TO 1
1303 IF(.NOT.TV.AND..NOT.UV.AND..NOT.SV) GO TO 304
VOL = .TRUE.
DO 1304 I=1,26
IF(RHO(I).NE.0.) VL(I) = 1./RHO(I)
IF(V(I).NE.0.) VL(I)=V(I)
IF(VL(I).EQ.0.) GO TO 1305
NP = I
1304 CCNTINUE
1305 TP = TV
HP = UV
SP = SV
GO TO 322
304 DO 305 I=1,26
IF(P(I).EQ.0.) GO TO 322
NP = I
IF (MMHG) P(NP) = P(NP)/760.
IF(PSIA ) P(NP)=P(NP)/14.696006
IF(NSCM) P(NP)=P(NP)/101325.
305 CONTINUE
322 DC 307 IT = 1,26
IF (T(IT).EQ.0.) GO TO 722
NT = IT
307 CCNTINUE
722 DO 625 IST=1,15
IF(WP(1).EQ.0.) OXF(IST)=0.
IF( MIX (IST).NE.0.) GO TO 323
IF(IST.NE.1) GO TO 745
WRITE(6,724)
724 FORMAT(48HONO INPT2 VALUE GIVEN FOR OF, EQRAT, FA, OR FPCT )
IF (WP(2).NE.0.) OXFL = WP(1)/WP(2)
GO TO 333
323 OXFL = MIX(IST)
IF(FA) OXFL =1./ MIX(IST)
IF(FPCT) OXFL =(100.- MIX(IST))/ MIX(IST)
IF(.NCT.ERATIO) GO TO 333
EQRAT = MIX(IST)
MAIN 157
MAIN 158
MAIN 159
MAIN 160
MAIN 161
MAIN 162
MAIN 163
MAIN 164
MAIN 165
MAIN 166
MAIN 167
MAIN 168
MAIN 169
MAIN 170
MAIN 171
MAIN 172
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MAIN 202
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MAIN 208
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MAIN 210
MAIN 211
MAIN 212
MAIN 213
MAIN 214

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IF(EQRAT.EQ.1.) EQRAT = 1.000005          MAIN 215
OXFL = (-EQRAT*VMIN(2)-VPLS(2))/(VPLS(1)+EQRAT*VMIN(1))   MAIN 216
333 OXF(IST) = OXFL                         MAIN 217
      NOF = IST                           MAIN 218
625 CONTINUE                                MAIN 219
745 IF (.NOT.IONS) GO TO 746                MAIN 220
      IF(LLMT(NLM).EQ.IE) GO TO 748        MAIN 221
      NLM = NLM+1                          MAIN 222
      LLMT(NLM) = IE                      MAIN 225
      BOP(NLM,1) = 0.                      MAIN 226
      BOP(NLM,2) = 0.                      MAIN 227
      GO TO 747                          MAIN 228
746 IF(LLMT(NLM).EQ.IE) NLM=NLM-1          MAIN 229
      NLM1 = NLM+1
      IF(LLMT(NLM1).NE.IE) GO TO 748
      LLMT(NLM1) = 0
747 NEWR = .TRUE.
      REWIND 4
748 IF(NEWR) CALL SEARCH
      IF(NS.EQ.0) GO TO 1                  MAIN 234
C
C      INITIAL ESTIMATES
C
      S0 = S0/R
      ENN = .1
      ENNL = -2.3025851
      SUMN = ENN
      XI = NS - NC
      XI = ENN/XI
      XLN = ALOG(XI)
      DO 432 J=1,NS
      IF(IUSE(J).GT.0) IUSE(J)=-IUSE(J)
      EN(J,1) = 0.
      ENLN(J) = 0.
      IF(IUSE(J).NE.0) GO TO 432
      EN(J,1) = XI
      ENLN(J) = XLN
432 CONTINUE
      IQ1 = NLM+1
      IF(NC.EQ.0.OR.NINSERT.EQ.0) GO TO 301
      DO 301 I=1,NINSERT
      INC = 0
      DO 301 J=1,NS
      IF(IUSE(J).EQ.0) GO TO 301
      INC = INC+1
      IF(SUB(J,1).NE.ENINSERT(1,I)) GO TO 301
      IF(SUB(J,2).NE.ENINSERT(2,I)) GO TO 301
      IF(SUB(J,3).NE.ENINSERT(3,I)) GO TO 301
      IF(T(1).EQ.0.) GO TO 295
      IF(T(1).LT.TEMP(INC,1).OR.T(1).GT.TEMP(INC,2)) GO TO 301
295  IQ1 = IQ1+1
      IUSE(J) = -IUSE(J)
301 CONTINUE
      IF(.NOT.TP.AND..NOT.HP.AND..NOT.SP) GO TO 800
      CALL THERMP
800  NINSERT = 0
      GO TO 1
2001 STOP
      END
                                         MAIN 235
                                         MAIN 236
                                         MAIN 237
                                         MAIN 238
                                         MAIN 239
                                         MAIN 240
                                         MAIN 241
                                         MAIN 242
                                         MAIN 243
                                         MAIN 244
                                         MAIN 245
                                         MAIN 246
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                                         MAIN 249
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                                         MAIN 280
                                         MAIN 281
                                         MAIN 282

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C      SUBROUTINE SEARCH                               SRCH   1
C      SEARCH TAPE FOR THERMO DATA FOR SPECIES TO BE CONSIDERED SRCH   2
C      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN           SRCH   3
C      INTEGER SUB,OMIT,END,TOOBIG                      SRCH   7
C      INTEGER SOLN                                     SRCH   8
C      LOGICAL NEWR,OTTO                            SRCH   9
C      LOGICAL NEWR,OTTO                            SRCH  10
C      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50) SRCH  11
C      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50) SRCH  12
C      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50) SRCH  13
C      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50) SRCH  14
C      DIMENSION DATE(2,3),MT(4),B(4),OMIT(3,3),NAM(3),TOOBIG(3,50) SRCH  15
C      COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250) MAIN  22
1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250) MAIN  23
COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) SRCH  18
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) SRCH  19
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5) SRCH  20
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) SRCH  21
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENN1,ENSAVE,ENLSAV,TRACE SRCH  22
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM SRCH  23
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFP,CPCVEQ SRCH  24
2 ,IONS,NC,INSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHSRCH 25
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM SRCH  26
COMMON/SOLN/SOLN(6,3),NSOLN SOLN   27
C      EQUIVALENCE (DATE,EN),(OMIT,ENLN),(ENDD,END),(TOOBIG,ENLN) SRCH  28
C      DATA GAS/1HG/,END/3HEND/ SRCH  29
C      DATA GAS/1HG/,END/3HEND/ SRCH  30
C      I2B = 0 SRCH  31
C      NC= 0 SRCH  32
C      IX= 0 SRCH  33
C      CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J) SRCH  34
C      CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J) SRCH  35
C      CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J) SRCH  36
C      CHECK DIMENSION FOR NUMBER OF SPECIES, CLEAR A(I,J) SRCH  37
C      DO 100 I=1,250 SRCH  38
C      DO 100 J=1,15 SRCH  39
100 A(J,I)=0.
SUB(1,1) = END SRCH  40
DO 3 I=1,1000 SRCH  41
IF(A(1,I).EQ.ENDD) GO TO 4 SRCH  42
DO 3 J=1,NLM SRCH  43
A(J,I) = 0. SRCH  44
3 CONTINUE SRCH  45
4 MAXNS = I-1 SRCH  46
C      READ TEMPERATURE RANGES FOR COEFFICIENTS OF GASEOUS SPECIES. SRCH  47
C      READ(4,5) TLOW,TMID,THIGH SRCH  48
5 FORMAT (3F10.3) SRCH  49
NS = 1 SRCH  50
C      BEGIN LOOP FOR READING SPECIES DATA FROM TAPE. SRCH  51
C      BEGIN LOOP FOR READING SPECIES DATA FROM TAPE. SRCH  52
C      BEGIN LOOP FOR READING SPECIES DATA FROM TAPE. SRCH  53
7 READ    (4,10)(NAM(I),I=1,3), DATE(1,NS),DATE(2,NS),(MT(J),B(J),SRCH  54
1 J=1,4),PHAZ,T1,T2 SRCH  55
10 FORMAT(3A4,6X,2A3,4(A2,F3.0),A1,2F10.3) SRCH  56

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IF(NAM(1).EQ.END)	GO TO 171	SRCH	57
READ	(4,20) ((COEF(I,J,NS),J=1,7),I=1,2)	SRCH	58
20 FORMAT (5E15.8)		SRCH	59
IF(NSOLN.EQ.0)	GO TO 200	SOLN	
DO 210 I=1,NSOLN		SOLN	
DO 230 J=1,3		SOLN	
IF(SOLN(J,I).NE.NAM(J))	GO TO 210	SOLN	
230 CONTINUE		SOLN	
IUSE(NS) = -999		SOLN	
GO TO 810		SOLN	
210 CONTINUE		SOLN	
200 CONTINUE		SOLN	
IF(NOMIT.EQ.0)	GO TO 810	SRCH	60
DC 805 I=1,NOMIT		SRCH	61
DO 804 J=1,3		SRCH	62
IF(OMIT(J,I).NE.NAM(J))	GO TO 805	SRCH	63
804 CONTINUE		SRCH	64
GO TO 7		SRCH	65
805 CONTINUE		SRCH	66
810 DO 820 K=1,4		SRCH	67
IF(B(K).EQ.0.)	GO TO 825	SRCH	68
DO 168 I=1,NLM		SRCH	69
IF(LLMT(I).EQ.MT(K))	GO TO 820	SRCH	70
168 CONTINUE		SRCH	71
IF(NS.GT.MAXNS)	GO TO 7	SRCH	72
DO 819 J=1,NLM		SRCH	73
819 A(J,NS) = 0.		SRCH	74
GO TO 7		SRCH	75
820 IF(NS.LE.MAXNS)	A(I,NS) = B(K)	SRCH	76
825 IF(NS.LE.MAXNS)	GO TO 828	SRCH	77
I2B = I2B+1		SRCH	78
DO 826 I=1,3		SRCH	79
826 TOOBIG(I,I2B) = NAM(I)		SRCH	80
GO TO 7		SRCH	81
828 DC 829 I=1,3		SRCH	82
829 SUB(NS,I) = NAM(I)		SRCH	83
IF(PHAZ.EQ.GAS)	IUSE(NS)=0	SRCH	85
IF(PHAZ.EQ.GAS)	GO TO 170	SRCH	86
C	NC= NC+1	SRCH	89
C	CONDENSED SPECIES	SRCH	88
TEMP(NC,1)= T1		SRCH	87
TEMP(NC,2)= T2		SRCH	90
IF(IUSE(NS).EQ.-999)	GOTO170	SRCH	91
IX= IX+1		SOLN	
IF(NS.EQ.1.OR.IUSE(NS-1).EQ.0.OR.IUSE(NS-1).EQ.-999)	GO TO 145	SRCH	92
DO 830 I=1,NLM		SOLN	
IF(A(I,NS).NE.A(I,NS-1))	GO TO 145	SRCH	94
830 CONTINUE		SRCH	95
IX= IX-1		SRCH	96
145 IUSE(NS)= -IX		SRCH	97
170 NS= NS+1		SRCH	98
GO TO 7		SRCH	99
C	END CARD HAS BEEN READ.	SRCH	100
C	171 NS= NS-1	SRCH	101
	NEWR= .FALSE.	SRCH	102
		SRCH	103
		SRCH	104
		SRCH	105

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      WRITE(6,172)                                     SRCH 106
172  FORMAT(42H0SPECIES BEING CONSIDERED IN THIS SYSTEM )   SRCH 107
      DO 174 I=1,NS,5                                SRCH 108
      I5= I+4                                         SRCH 109
      IF(NS.LT.I5) I5=NS                            SRCH 110
174  WRITE (6,176) (DATE(1,J),DATE(2,J),SUB(J,1),SUB(J,2),SUB(J,3),J=I,
1    I5)                                         SRCH 111
176  FORMAT(5(5X,2A3,2X,3A4))                     SRCH 112
      IF(NSOLN.EQ.0) GO TO 220                      SOLN
      PRINT1000, ((SOLN(J,I),J=1,3),I=1,NSOLN)     SOLN
1000 FORMAT('0SELECTED COMPONENTS FOR SOLUTION PHASE ARE:',2(3X,3A4)) SOLN
220  CCONTINUE                                      SOLN
      IF(I2B.GT.0) GO TO 870                         SPCH 114
      RETURN                                         SRCH 115
870  WRITE(6,871) I2B                               SRCH 116
871  FORMAT(35H0INSUFFICIENT STORAGE FOR FOLLOWING,I3,8H SPECIES) SRCH 117
      WRITE(6,880) (TOOBIG(1,J),TOOBIG(2,J),TOCBIG(3,J),J=1,I2B) SRCH 118
880  FORMAT(8(3X,3A4))                           SRCH 119
      NS = 0                                         SRCH 120
      RETURN                                         SRCH 121
      END                                            SRCH 122
      SUBROUTINE EQLBRM                           EQLM  1
C   ROUTINE TO CALCULATE EQUILIBRIUM COMPOSITION AND PROPERTIES EQLM  2
C
      DOUBLE PRECISION X,G,SUM,SUM2,E                 EQLM0004
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS   EQLM  9
      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN          EQLM 10
      DOUBLE PRECISION ENL,PROW,DINT,AA               EQLM 11
      DOUBLE PRECISION EN10,EN20,C1,C2                SOLN
C
      LOGICAL HP,SP,TP,CONVG,IONS,SINGC,LOGV,ISING,I35,VOL,SHOCK,RITE EQLM 12
C
C
      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) EQLM 16
2 ,VLM(13),TOTN(13)                                         EQLM 17
      COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250) MAIN 22
1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250) MAIN 23
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) EQLM 21
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) EQLM 22
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        EQLM 23
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) EQLM 24
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENN,LNSAVE,ENLSAV,TRACE,SIZE       EQLM 25
      COMMON /DOUBLE/ G(20,21), X(20)                  EQLM 26
      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM EQLM 27
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ EQLM 28
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHEQLM 29
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM                         EQLM 30
      COMMON/IS/IS,JSOL1,JSOL2                         SOLN
      COMMON/COMP/EN10,EN20,C1,C2                       SOLN
C
      EQUIVALENCE (NLM,L),(LOGV,CPCVEQ)             EQLM 31
C
      DATA IE/1HE/,SMALNO/1.E-6/,SMNOL/-13.815511/,ITN/35/           EQLM 32
C
      CALL ERRSET(263,256,256,1)                      EQLM 33
      SINGC = .FALSE.                                 EQLM 34
      PIE = 0.                                       EQLM 35
      I35 = .FALSE.                                 EQLM 36

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E = 2.718281828459
ENL = ENNL 37
RITE = .FALSE.
IF (IDEBUG.GT.0.AND.NPT.GE.IDEBUG) RITE=.TRUE.
ISING = .FALSE.
LOGV = .FALSE.
IF (.NOT.VOL) GO TO 6
RV = RR/101.325
PP = RV*ENN*TT/VLM(NPT)
6 TLN = ALOG(TT)
CONVG = .FALSE.
ITNUMB = ITN
JS1 = 1
CALL CPHS
TM = ALOG(PP/ENN)
C
      IF (.NOT.IONS.OR.IE.EQ.LLMT(L)) GO TO 33
      L = L+1
      IQ1 = IQ1+1
      DC 499 J = 1,NS
      IF (A(L,J) -EQ-0-) GO TO 499
      EN(J,NPT) = 1.E-8
      ENLN(J) = -SIZE
      499 CONTINUE
      33 IF (NPT.EQ.1.AND..NOT.SHOCK)          WRITE(6,244) (LLMT(I),I=1,L)
      244 FORMAT (4H0PT ,14(5X,A4))
C
C     BEGIN ITERATION
C
      43 IF (.NOT.CONVG) GO TO 62
      SUMN = ENN
      IF (JSOL.EQ.0) GO TO 62
      ENSOL = EN(JSOL,NPT)
      EN(JSOL,NPT) = EN(JSOL,NPT)+EN(JLIQ,NPT)
      IUSE(JLIQ) = -IUSE(JLIQ)
      IQ1 = IQ1-1
      DLVTP(NPT) = 0.
      CPR(NPT) = 0.
      GAMMAS(NPT) = 0.
      LOGV = .TRUE.
      62 CONTINUE
      CALL MATRIX
      NUMB = ITN-ITNUMB+1
      IF (NUMB.GT.16) RITE=.TRUE.
      IQ2 = IQ1 + 1
      IF (CONVG) IMAT=IMAT-1
      IF (.NOT.RITE) GO TO 72
      IF (.NOT.CONVG) GO TO 88
      IF (.NOT.LOGV) WRITE(6,81)
      81 FCORMAT(15H0T DERIV MATRIX)
      IF (LOGV) WRITE(6,82)
      82 FORMAT(15H0P DERIV MATRIX)
      GO TO 89
      88 WRITE(6,772) NUMB
      772 FORMAT (11H0ITERATION ,I3,6X,7HMATRIX //)
      89 DO 911 I=1,IMAT
      911 WRITE (6,73) (G(I,K),K=1,KMAT)
      72 ITST = IMAT
      CALL GAUSS
      EQLM 38
      EQLM 39
      EQLM 41
      EQLM 42
      EQLM 43
      EQLM 44
      EQLM 45
      EQLM 46
      EQLM 47
      EQLM 48
      EQLM 49
      EQLM 50
      EQLM 51
      EQLM 52
      EQLM 53
      EQLM 54
      EQLM 55
      EQLM 56
      EQLM 57
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      EQLM 59
      EQLM 61
      EQLM 62
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      EQLM 64
      EQLM 65
      EQLM 66
      EQLM 67
      EQLM 68
      EQLM 69
      EQLM 70
      EQLM 71
      EQLM 72
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      EQLM 79
      EQLM 80
      EQLM 81
      EQLM 82
      EQLM 83
      EQLM 84
      EQLM 85
      EQLM 86
      EQLM 87
      EQLM 88
      EQLM 89
      EQLM 90
      EQLM 91
      SQLM 92
      EQLM 93
      EQLM 94

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IF(ITST.NE.IMAT) GO TO 774          EQLM  95
IF(.NOT.RITE)   GO TO 773          EQLM  96
WRITE(6,373)(LLMT(I),I=1,L)        EQLM  97
373 FORMAT(7H0PI ,9(A4,10X))       EQLM  98
WRITE(6,73)(X(I),I=1,IMAT)        EQLM  99
73 FORMAT(1X,1P12E11.3)
773 IF(.NOT.CONVG) GO TO 85        SOLN
IF(-NCT.LOGV)   GO TO 174          EQLM 101
GO TO 171                          EQLM 102
C                                     EQLM 103
C                                     EQLM 104
C                                     TEMPERATURE DERIVATIVES--CONVG=T, LOGV=F
C                                     EQLM 105
C                                     EQLM 106
C                                     EQLM 107
174 DLVTP(NPT) = 1.-X(IQ1)
IF(DLVTP(NPT).LT.25.) GO TO 175
DLVTP(NPT) = 0.
DLVPT(NPT) = 0.
CPR(NPT) = 0.
GAMMAS(NPT) = 0.
GO TO 186
175 CPR(NPT) = G(IQ2,IQ2)          EQLM 108
DO 176 J=1,IQ1
CPR(NPT) = CPR(NPT)-G(IQ2,J)*X(J)
176 CCNTINUE                         EQLM 109
C                                     EQLM 110
C                                     EQLM 111
C                                     EQLM 112
C                                     EQLM 113
C                                     EQLM 114
LOGV = .TRUE.                         EQLM 115
GO TO 62                            EQLM 116
C                                     EQLM 117
C                                     EQLM 118
C                                     EQLM 119
774 IF(.NOT.CONVG) GO TO 775          EQLM 120
WRITE(6,172)                         EQLM 121
172 FORMAT(28H0DERIVATIVE MATRIX SINGULAR )
GC TO 1171                           EQLM 122
EQLM 123
775 IF(.NCT.HP.OR.NPT.NE.1.OR.NC.EQ.0.OR.TT.GT.100.) GO TO 871
WRITE(6,874)                         EQLM 124
EQLM 125
874 FORMAT(96H0LOW TEMPERATURE IMPLIES CONDENSED SPECIES SHOULD HAVE
1BEEN INCLUDED ON AN INSERT CARD, RESTART )          EQLM 126
GO TO 873                           EQLM 127
EQLM 128
871 WRITE(6,74)                      EQLM 129
74 FORMAT(16H0SINGULAR MATRIX)        EQLM 130
IF(SINGC) GO TO 873
DO 970 JJ = 1, NS
IF(IUSE(JJ).NE.0) GO TO 970
IF(EN(JJ,NPT).NE.0.) GO TO 970
EN(JJ,NPT) = SMALNO
ENLN(JJ) = SMNOL
970 CONTINUE                         EQLM 131
IF(ISING) GO TO 870
ISING = .TRUE.
WRITE(6,776)                         EQLM 132
EQLM 133
776 FCRMAT(8H0RESTART)              EQLM 134
GO TO 62                            EQLM 135
EQLM 136
C                                     EQLM 137
C                                     EQLM 138
C                                     EQLM 139
TEST FOR SINGULARITY TO CONDENSED SPECIES.          EQLM 140
C                                     EQLM 141
C                                     EQLM 142
C                                     EQLM 143
870 NCOND = IQ1-NLM-2                EQLM 144
IF(TP.OR.VOL) NCOND=NCOND+1          EQLM 145
EQLM 146

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IF(NCOND.LT.2.OR.SIZEG.EQ.0.) GO TO 873          EQLM 148
DO 872 J=1,NS          EQLM 149
IF(IUSE(J).LE.0) GO TO 872          EQLM 150
IF(J.EQ.JDELG) GO TO 872          EQLM 151
DO 671 I=1,NLM          EQLM 152
IF(A(I,J).EQ.A(I,JDELG)) GO TO 671          EQLM 153
IF(A(I,J).EQ.0..OR.A(I,JDELG).EQ.0.) GO TO 872          EQLM 154
671 CONTINUE          EQLM 155
SINGC = .TRUE.          EQLM 156
IQ1 = IQ1-1          EQLM 157
EN(J,NPT) = 0.          EQLM 158
IUSE(J) = -IUSE(J)          EQLM 159
872 CONTINUE          EQLM 160
IF(SINGC) GO TO 40          EQLM 161
GC TO 873          EQLM 162
C OBTAIN CORRECTIONS TO THE ESTIMATES          EQLM 163
C
85 ITNUMB= ITNUMB-1          EQLM 164
KK = L + 1          EQLM 165
IF(VOL) X(IQ2)=X(IQ1)          EQLM 166
IF(TP) X(IQ2)=0.          EQLM 167
DLNT= X(IQ2)          EQLM 168
SUM = X(IQ1)          EQLM 169
IF(.NOT.VOL) GO TO 97          EQLM 170
X(IQ1) = 0.          EQLM 171
SUM = -DLNT          EQLM 172
97 DO 101 J=1,NS          EQLM 173
IF (IUSE(J)) 101,98,100          EQLM 174
98 DELN(J) = H0(J)*DLNT-H0(J)+S(J)-ENLN(J)-TM+SUM          EQLM 175
DO 99 K=1,L          EQLM 176
DELN(J) = DELN(J)+A(K,J)*X(K)          EQLM 177
99 CONTINUE          EQLM 178
IF(PIE.NE.0.) DELN(J)=DELN(J)+A(L+1,J)*PIE          EQLM 179
GO TO 101          EQLM 180
100 DELN(J) = X(KK)          EQLM 181
KK = KK + 1          EQLM 182
101 CONTINUE          EQLM 183
C CALCULATE CONTROL FACTOR,AMBDA          EQLM 184
C
AMBDA= 1.          EQLM 185
AMBDA1= 1.          EQLM 186
SUM = X(IQ1)          EQLM 187
IF(SUM.LT.0.) SUM=-SUM          EQLM 188
IF(DLNT.GT.SUM) SUM=DLNT          EQLM 189
IF(-DLNT.GT.SUM) SUM=-DLNT          EQLM 190
DO 917 J=1,NS          EQLM 191
IF (IUSE(J).NE.0) GO TO 917          EQLM 192
IF((EN(J,NPT).GT.0.).AND.DELN(J).GT.SUM) SUM = DELN(J)          EQLM 193
IF((EN(J,NPT).NE.0.) .OR. DELN(J).LE.0.) GO TO 917          EQLM 194
SUM1 = (-9.212-ENLN(J) + ENL)/(DELN(J)-X(IQ1))          EQLM 195
IF(SUM1.LT.0.) SUM1=-SUM1          EQLM 196
IF (SUM1.LT.AMBDA1) AMBDA1 = SUM1          EQLM 197
917 CONTINUE          EQLM 198
IF(SUM.GT.2.) AMBDA=2./SUM          EQLM 199
IF (AMBDA1.LT.AMBDA) AMBDA = AMBDA1          EQLM 200
IF(.NOT.RITE) GO TO 111          EQLM 201
C

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C      INTERMEDIATE OUTPUT                           EQLM 206
C
C      WRITE(6,923) TT,ENN,ENL,PP,TM,AMBDA          EQLM 207
923 FORMAT(3H0T=,E15.8,6H ENN=,E15.8,7H ENNL=E15.8,5H PP=,E15.8,    EQLM 208
   1 9H LN P/N=E15.8,8H AMEDA=E15.8 )           EQLM 209
   IF(VOL) WRITE(6,1924) VLM(NPT)                EQLM 210
1924 FORMAT(8H VOLUME=,E15.8,4HCC/G)            EQLM 211
   WRITE(6,924)                                     EQLM 212
924 FORMAT(1H0,18X,2HNJ,12X,5HLN NJ,8X,9HDEL LN NJ,9X,6HH0J/RT,9X,5HS0EQLM 214
   1J/R,10X,7H-GOJ/RT,8X,6H-GJ/RT )             EQLM 215
   DO 926 J=1,NS                                EQLM 216
   GNEG1 = S(J)-H0(J)                            EQLM 217
   GNEG2 = GNEG1                                EQLM 218
   IF(IUSE(J).EQ.0) GNEG2=GNEG2-ENLN(J)-TM     EQLM 219
   WRITE(6,925) SUB(J,1),SUB(J,2),               EQLM 220
   1SUB(J,3),EN(J,NPT),ENLN(J),DELN(J),H0(J),S(J),GNEG1,GNEG2
925 FORMAT(1X,3A4,7E15.6)                        EQLM 221
926 CONTINUE                                     EQLM 222
   WRITE(6,110)                                    EQLM 223
110 FORMAT(1H0)                                   EQLM 224
C
C      APPLY CORRECTIONS TO ESTIMATES            EQLM 225
C
C      111 SUM = 0.                               EQLM 226
C      IF(AMBDA.LT..1.AND.IS.NE.0) AMBDA=.1       EQLM 227
DO 113 J=1,NS                                EQLM 228
   IF(IUSE(J)) 113,112,114                      EQLM 229
112 ENLN(J)=ENLN(J)+AMBDA*DELN(J)            EQLM 230
   EN(J,NPT) = 0.                                EQLM 231
   IF((ENLN(J)-ENL+SIZE).LE.0.) GO TO 113        EQLM 232
   EN(J,NPT) = E**ENLN(J)                         EQLM 233
   SUM = SUM+EN(J,NPT)                          EQLM 234
   GO TO 113                                     EQLM 235
114 EN(J,NPT) = EN(J,NPT) + AMBDA * DELN(J)    EQLM 236
113 CONTINUE                                     EQLM 237
   ISKIP = 1
   IF(ISKIP.EQ.1) GOTO510
   IF(IS.EQ.0) GOTO510
   IF(EN(JSOL1,NPT).LT.0.D0) EN(JSOL1,NPT)=1.D-12
   IF(EN(JSOL2,NPT).LT.0.D0) EN(JSOL2,NPT)=1.D-12
510 CONTINUE                                     SOLN
   SUMN = SUM
   IF(TP) GO TO 115
   TLN= TLN+AMBDA*DLNT
   TT = EXP(TLN)
   JS1 = 1
   CALL CPHS
115 IF(VOL) GO TO 2115
   ENL = ENL+AMBDA*X(IQ1)
   ENN = E**ENN
   GO TO 1115
2115 ENN = SUMN
   ENL = ALOG(ENN)
   PP = RV*TT*ENN/VLM(NPT)
1115 TM = ALOG(PP/ENN)
   IF(LLMT(I).NE.IE) GO TO 116
C
C      CHECK ON REMOVING IONS                   EQLM 240
C

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DO 1116 J = 1,NS          EQLM 258
IF (A(L,J).EQ.0.) GO TO 1116   EQLM 259
IF (EN(J,NPT).GT.0.) GO TO 116   EQLM 260
1116 CONTINUE             EQLM 261
    PIE = X(L)
    L = L-1
    IQ1 = IQ1-1
    GO TO 43
C
C      TEST FOR CONVERGENCE
C
116 IF (ITNUMB.EQ.0) GO TO 14
IF (AMBDA.LT.1.) GO TO 43
SUM = X(IQ1)
IF (SUM.LT.0.) SUM = -SUM
IF (SUM.GT.0.5E-5) GO TO 43
DO 130 J=1,NS
IF (IUSE(J).LT.0) GO TO 130
AA= DELN(J)/SUMN
IF (AA.LT.0.) AA=-AA
IF (IUSE(J).EQ.0) AA = AA*EN(J,NPT)
IF (AA.GT.0.5E-5) GO TO 43
130 CONTINUE
LE = L
IF(TRACE.EQ.0.) GO TO 275
IF(ITN.GT.35) GO TO 222
ITN = ITN+15
ITNUMB = ITNUMB+15
222 DO 225 I=1,NLM
IF(B0(I).EQ.0.) GO TO 227
SUM = 0.
DO 223 J=1,NS
223 SUM = SUM+EN(J,NPT)*A(I,J)
TSUM = SUM
EPS = ABS(B0(I)-TSUM)/B0(I)
IF(ABS(B0(I)-TSUM)/B0(I).GT..0001) GO TO 43
225 CONTINUE
227 IF(.NOT.IONS) GO TO 275
C
C      CHECK ON ELECTRON BALANCE
C
    IF(PIE.NE.0.) LE=L+1
    IF(PIE.EQ.0.) PIE=X(L)
    ITER = 1
229 SUM2 = 0.
    SUM = 0.
    DO 230 J=1,NS
    IF(IUSE(J).LT.0.OR.A(LE,J).EQ.0.) GO TO 230
    IF(ENLN(J).GT.-.87.) EN(J,NPT)=E**ENLN(J)
    AN = A(LE,J)*EN(J,NPT)
    IF(EN(J,NPT)/ENN.GT.1.E-7) GO TO 275
    SUM = SUM+AN
    SUM2 = SUM2+AN*A(LE,J)
230 CONTINUE
    IF(SUM2.EQ.0.) GO TO 275
    DPIE = -SUM/SUM2
    DO 250 J=1,NS
    IF(A(LE,J).EQ.0.) GO TO 250
    ENLN(J) = ENLN(J)+A(LE,J)*DPIE

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250 CONTINUE
  IF(ABS(DPIE).LE..0001) GO TO 275
  PIE = PIE+DPIE
  ITER = ITER+1
  IF(ITER.LE.ITN) GO TO 229
  WRITE(6,260)
260 FORMAT(37HODID NOT CONVERGE ON ELECTRON BALANCE)
  GC TO 873
275 CONTINUE
C
C      CALCULATE ENTROPY, CHECK ON DELTA S FOR SP PROBLEMS
C
C      TOTN(NPT) = 0.
C      SSUM(NPT) = 0.
C      DO 183 J=1,NS
C      IF(IUSE(J).LT.0) GO TO 183
C      TCTN(NPT) = TOTN(NPT) + EN(J,NPT)
C      SS = S(J)
C      IF(IUSE(J).EQ.0) SS=SS-ENLN(J)-TM
C      SSUM(NPT) = SSUM(NPT)+SS*EN(J,NPT)
183 CONTINUE
  IF(.NOT.SP) GO TO 13
  SS = SSUM(NPT) -SO
  IF(SS.LT.(-0.00005).OR.SS.GT.0.00005) GO TO 43
  IF(RITE) WRITE(6,1183) SS
1183 FORMAT(12HODELTA S/R =,E15.8)
C
C      13 CONVG=.TRUE.
C      GO TO 160
C      14 WRITE(6,973) ITN,NPT
973 FORMAT(1HL,I2,69H ITERATIONS DID NOT SATISFY CONVERGENCE REQUIREMENT)
C      1NTS FCR THE POINT I5)
C      IF(NC.EQ.0.OR.I35) GO TO 873
C      I35 = .TRUE.
C      IF (.NOT.HP.OR.NPT.NE.1.OR.TT.GT.100.) GO TO 261
C      WRITE(6,874)
C      GO TO 873
261 NCOND = IQ1-NLM-2
  IF(TP.OR.VOL) NCOND=NCOND+1
  IF(NCOND.NE.1.OR.ENN.GT.1.E-4) GO TO 873
C      HIGH TEMPERATURE, INCLUDED CONDENSED CONDITION
  WRITE(6,265)
265 FORMAT(31HOTRY REMOVING CONDENSED SPECIES)
  ENN = .1
  ENL = -2.3025851
  SUMN = ENN
  XI = NS - NC
  XI = ENN/XI
  XLN = ALOG(XI)
  DO 432 J=1,NS
    IF(IUSE(J).GT.0) IUSE(J)=-IUSE(J)
    EN(J,NPT) = 0.
    ENLN(J) = 0.
    IF (IUSE(J).NE.0) GO TO 432
    EN(J,NPT) = XI
    ENLN(J) = XLN
432 CONTINUE
  IQ1 = NLM+1
  GO TO 40

```

C CONVERGENCE TESTS ARE SATISFIED, TEST CONDENSED SPECIES.

C

160 IF(NC.EQ.0) GO TO 143 EQLM 309
 DO 146 J=1,NS EQLM 310
 IF(EN(J,NPT).GE.0.) GO TO 146 EQLM 311
 IF (J.NE.JSOL .AND. J .NE.JLIQ) GO TO 147 EQLM 312
 JSOL = 0 EQLM 313
 JLIQ = 0 EQLM 314
 147 IQ1 = IQ1 - 1 EQLM 315
 EN(J,NPT) = 0. EQLM 316
 GO TO 166 EQLM 317
 146 CONTINUE EQLM 318
 SIZEG = 0. EQLM 319
 INC = 0 EQLM 320
 DO 170 J = 1,NS EQLM 321
 IF(IUSE(J).EQ.0) GO TO 170 EQLM 322
 INC = INC + 1 EQLM 323
 IF(RITE) WRITE(6,144)(SUB(J,I),I=1,3),TEMP(INC,1),TEMP(INC,2),IUSE,1E(J),EN(J,NPT) EQLM 324
 144 FORMAT (1H0,3A4,2F10.3,3X,5HIUSE=,I4,E15.7) EQLM 325
 IF(IUSE(J).LT.-900) GOT0170 SOLN
 IF(EN(J,NPT).GT.0.) GO TO 169 EQLM 326
 KG = 1 EQLM 327
 IF(IUSE(J).EQ.-IUSE(J+1)) GO TO 154 EQLM 328
 IF(J.EQ.1.OR.IUSE(J).NE.-IUSE(J-1)) GO TO 153 EQLM 329
 KG = -1 EQLM 330
 154 JKKG = J + KG EQLM 331
 TMELT = TEMP(INC,1) EQLM 332
 IMP = INC + KG EQLM 333
 IF(TMELT.EQ.TEMP(IMP,2)) GO TO 158 EQLM 334
 TMELT = TEMP(INC,2) EQLM 335
 IF (TMELT.EQ.TEMP(IMP,1)) GO TO 157 EQLM 336
 WRITE (6,156) EQLM 337
 156 FORMAT (50H03 PHASES OF A CONDENSED SPECIES ARE OUT OF ORDER) EQLM 338
 GO TO 873 EQLM 339

C JTH SPECIES A SOLID (EN=0), (J+KG) TH SPECIES A LIQUID (EN IS +)

C

157 IF(TT.GT.TMELT) GO TO 169 EQLM 340
 IF (TP.AND.TT.EQ.TMELT) GO TO 169 EQLM 341
 IF (TP) GO TO 1165 EQLM 342
 IF (TT.LE.TMELT-150.) GO TO 1165 EQLM 343
 JSOL = J EQLM 344
 JLIQ = JKKG EQLM 345
 GO TO 159 EQLM 346

C JTH SPECIES A LIQUID(EN=0), (J+KG) TH SPECIES A SOLID (EN IS +)

C

158 IF (TI.LT.TMELT) GO TO 169 EQLM 347
 IF (TP.AND.TT.EQ.TMELT) GO TO 169 EQLM 348
 IF (TP) GO TO 1165 EQLM 349
 IF (TT.GE.TMELT+150.) GO TO 1165 EQLM 350
 JSOL = JKKG EQLM 351
 JLIQ = J EQLM 352
 GO TO 159 EQLM 353

159 TLN = ALOG (TMELT) EQLM 354
 TI = TMELT EQLM 355
 EN(JKG,NPT) = .5 * EN(JKG,NPT) EQLM 356
 EN(J,NPT) = EN(JKG,NPT) EQLM 357
 EN(J,NPT) = EN(JKG,NPT) EQLM 358
 EN(J,NPT) = EN(JKG,NPT) EQLM 359
 EN(J,NPT) = EN(JKG,NPT) EQLM 360
 EN(J,NPT) = EN(JKG,NPT) EQLM 361
 EN(J,NPT) = EN(JKG,NPT) EQLM 362
 EN(J,NPT) = EN(JKG,NPT) EQLM 363
 EN(J,NPT) = EN(JKG,NPT) EQLM 364
 EN(J,NPT) = EN(JKG,NPT) EQLM 365
 EN(J,NPT) = EN(JKG,NPT) EQLM 366

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GC TO 165                                EQLM 367
C
C   WRONG PHASE INCLUDED FOR T INTERVAL, SWITCH EN      EQLM 368
C
C
1165 EN(J,NPT) = EN (JKG, NPT)          EQLM 369
    IUSE(J) = -IUSE(J)                  EQLM 370
    IUSE (JKG) = -IUSE(JKG)           EQLM 371
    EN(JKG,NPT)= 0.                   EQLM 372
    GO TO 40                           EQLM 373
153 IF (TT.LT.TEMP(INC,1) .AND.TEMP(INC,1).NE.TLOW) GO TO 169 EQLM 374
    IF (TT.GT.TEMP(INC,2)) GO TO 169 EQLM 375
C
C
SUM = 0.                                     EQLM 376
DO 167 I = 1,L                            EQLM 377
    SUM = SUM + A(I,J)*X(I)             EQLM 378
167 CONTINUE                               EQLM 379
    IUSE (J) = -IUSE (J)                EQLM 380
    JS1 = 1                             SOLN
    CALL CPHS                          SOLN
    IUSE (J) == IUSE (J)                SOLN
    DELG = H0 (J)-S(J)-SUM            EQLM 381
    IF(RITE)  WRITE(6,168)DELG,SIZEG EQLM 382
168 FORMAT (18H GO-SUM(AIJ*PII) =E15.7,10X,17HMAX NEG DELTA G =,E15.7) EQLM 383
    IF(DELG.GE.SIZEG .OR. DELG.GE.0.) GO TO 169 EQLM 384
    SIZEG = DELG                      EQLM 385
    JDELG = J                         EQLM 386
169 IF(INC.EQ.NC) GO TO 1160              EQLM 387
170 CONTINUE                               EQLM 388
1160 IF (SIZEG.EQ.0.) GO TO 143          EQLM 389
    J = JDELG
165 IQ1 = IQ1 + 1                         EQLM 390
166 IUSE (J) = - IUSE (J)                EQLM 391
40 CONVG = .FALSE.                      EQLM 392
    JS1 = 1                             EQLM 393
    CALL CPHS                          EQLM 394
143 TN = NUMB                            EQLM 395
    IF(PIE.NE.0.) X(LE) = PIE
770 IF(.NOT.SHOCK)          WRITE(6,771)NPT,(X(IL),IL=1,LE),TN EQLM 396
771 FORMAT (I3,14F9.3)                  EQLM 397
    JS1 = 1
    IF(TP.AND.CONVG) CALL CPHS        EQLM 398
    ITNUMB = ITN
    IF(.NOT.CONVG.OR.IS.NE.0) GOTO43 EQLM 399
    CONVG = .FALSE.
    IS = 1
    IQ1 = IQ1+2
    JSOL1 = 0
    INC = 0
    DO 500 J=1,NS
    IF(IUSE(J).EQ.0) GOTO500
    INC = INC+1
    IF(IUSE(J).GT.-900) GOTO500
    IF(TT.LE.TEMP(INC,1).OR.TT.GT.TEMP(INC,2)) GOTO500
    IUSE (J) = 999
    IF(JSOL1.EQ.0) JSOL1=J
    IF(JSOL1.NE.0) JSOL2=J
500 CONTINUE
    EN(JSOL1,NPT) = EN10

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EN(JSOL2,NPT) = EN20          SOLN
JS1 = 1                      SOLN
CALL CPHS                     SOLN
GO TO 43                      EQLM 405
C
C      CALCULATE EQUILIBRIUM PROPERTIES
C
C
1171 DLVPT(NPT) = -1.          EQLM 406
    DLVTP(NPT) = 1.             EQLM 406
    CPR(NPT) = CPSUM           EQLM 407
    GO TO 199                  EQLM 407
171  DLVPT(NPT) = -1. + X(IQ1)  EQLM 408
    IF(JLIQ.EQ.0) GO TO 199    EQLM 408
    EN(JSOL,NPT) = ENSOL       EQLM 409
    IUSE(JLIQ) = -IUSE(JLIQ)   EQLM 409
    HSUM(NPT) = HSUM(NPT) + EN(JSOL,NPT)*(H0(JLIQ)-H0(JSOL))  EQLM 410
    IQ1 = IQ1+1                 EQLM 411
    GAMMAS(NPT) = -1./DLVPT(NPT)  EQLM 412
    GO TO 186                  EQLM 413
199  GAMMAS(NPT) = -1./(DLVPT(NPT)+(DLVTP(NPT)**2)*ENN/CPR(NPT))  EQLM 414
'186 TTT(NPT) = TT            EQLM 415
    ENNL = ENL                  EQLM 416
    PPP(NPT) = PP                EQLM 417
    VLM(NPT) = RR*ENN*TT/(101.325*PP)  EQLM 418
    HSUM(NPT) = HSUM(NPT)*TT      EQLM 419
    WM(NPT) = 1./ENN             EQLM 420
    IF(TRACE.EQ.0.) GO TO 200    EQLM 421
    DO 1200 J=1,NS              EQLM 422
    IF(IUSE(J).NE.0) GO TO 1200  EQLM 423
    IF(ENLN(J).GT.-87.) EN(J,NPT)=E**ENLN(J)  EQLM 424
1200 CONTINUE                   EQLM 425
200  IF(.NOT.RITE) GO TO 863    EQLM 426
    WRITE(6,201) NPT,             PP,TT,HSUM(NPT),SSUM(NPT),WM(NPT),CPR(NPEQLM 427
    1T),DLVPT(NPT),DLVTP(NPT),GAMMAS(NPT),VLM(NPT)  EQLM 428
201  FORMAT(7H0POINT=I3,3X,2HP=E13.6,3X,2HT=E13.6,3X,4HH/R=E13.6,3X,4HEQLM 429
    1S/R=E13.6//3X,3HMW=E13.6,3X,5HCP/R=E13.6,3X,6HDLVPT=E13.6,3X,6HDLVEQLM 430
    2TP=E13.6,3X,9HGAMMA(S)=E13.6,3X,2HV=,E13.6)  EQLM 431
863  IF(TT.GE.TLOW.AND.TT.LE.THIGH.OR.SHOCK) GO TO 1000  EQLM 432
    WRITE(6,306) TT,NPT          EQLM 433
306  FORMAT(17H0THE TEMPERATURE=E12.4,26H IS OUT OF RANGE FOR POINT,I5)  EQLM 434
    IF(TT.GE.TLOW/1.5.AND.TT.LE.THIGH*1.25) GO TO 1000  EQLM 435
    NPT = NPT+1                  EQLM 436
C
C      ERROR, SET TT=0
C
873  TT=0.
    NPT = NPT-1                 EQLM 437
1000 RETURN                     EQLM 438
    END                         EQLM 439
C
C      SUBROUTINE REACT
C
C      LOGICAL HP,SP,TP,           CONVG,NEWR,IONS,MOLES,EQL,FROZ,VOL  REAC 1
C
C      DIMENSION ANAME(15,5),V(15),LLMTS(15),SBOP(15,2)  REAC 2
C
C      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)  REAC 3
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) REAC 4

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2 ,HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5) REAC 9
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) REAC 10
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE,SIZE REAC 11
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM REAC 12
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ REAC 13
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHREAC 14
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM REAC 15
C
C      EQUIVALENCE (NAME,ANAME),(NLM,L),(BLANK,LANK) REAC 16
C
C      DATA MOL/1HM/,OX/1HO/,LANK/1H /,IZERO/2H00/,NLS/0/,ZERO/1HO/ REAC 19
C
C      DC 10 K=1,2 REAC 21
C      WP(K)=0. REAC 22
C      HPP(K)=0. REAC 23
C      RH(K)=0. REAC 24
C      VPLS(K)=0. REAC 25
C      VMIN(K)=0. REAC 26
C      AM(K)=0. REAC 27
C      DO 8 J=1,15 REAC 28
C      LLMT(J)=0 REAC 29
C      BOP(J,K)=0. REAC 30
C      8 CONTINUE REAC 31
C      10 CONTINUE REAC 32
C      NFUEL = 0 REAC 33
C      N=1 REAC 34
C      L=1 REAC 35
C
C      READ AND WRITE REACTANT CARDS REAC 36
C
C      20 READ(5,21)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ(N) REAC 39
C      1 ,RTEMP(N),FOX(N),DENS(N) REAC 40
C      21 FORMAT(5(A2,F7.5),F7.5,A1,F9.5,A1,F8.5,A1,F8.5) REAC 41
C      IF(NAME(N,1).EQ.LANK) GO TO 200 REAC 42
C      IF(L.EQ.0) GO TO 20 REAC 43
C      WRITE (6,31)(NAME(N,I),ANUM(N,I),I=1,5),PECWT(N),MOLE,ENTH(N),FAZ REAC 44
C      1 (N),RTEMP(N),FOX(N),DENS(N) REAC 45
C      31 FORMAT(1X,5(A2,1X,F7.4,2X),F10.6,2X,A1,F11.2,2X,A1,2X,F8.3,2X, REAC 46
C      1A1,3X,F8.5) REAC 47
C      35 IF(MOLE.EQ.MOL) MOLES=.TRUE. REAC 48
C
C      IF OXIDANT, K=1 REAC 49
C      IF FUEL, K=2 REAC 50
C
C      IF(FOX(N).EQ.ZERO) FOX(N)=OX REAC 53
C      K = 1 REAC 54
C      IF(FOX(N).EQ.OX) GO TO 37 REAC 55
C      K = 2 REAC 56
C      NFUEL = NFUEL+1 REAC 57
C      37 DO 38 J=1,15 REAC 58
C      DATA(J) = 0. REAC 59
C      38 CONTINUE REAC 60
C      RM=0. REAC 61
C
C      STORE ATOMIC SYMBOLS IN LLMT ARRAY. REAC 62
C      CALCULATE MOLECULAR WEIGHT. REAC 63
C      TEMPORARILY STORE ATOMIC VALENCE IN V. REAC 64
C
C      DO 100 JJ=1,5 REAC 65
C
C

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IF(ANUM(N,JJ).EQ.0.) GO TO 101          REAC  68
IF(ANAME(N,JJ).EQ.ZERO) ANAME(N,JJ)=OX   REAC  69
DO 41 J=1,15                            REAC  70
NJ = J                                 REAC  71
IF(LLMT(J).EQ.0) GO TO 45              REAC  72
IF(NAME(N,JJ).EQ.LLMT(J)) GO TO 46      REAC  73
41 CONTINUE                            REAC  74
45 L = NJ                               REAC  75
LLMT(J)=NAME(N,JJ)                     REAC  76
46 DO 48 KK=1,101                      REAC  77
IF(ATOM(1,KK).EQ.ANAME(N,JJ)) GO TO 50  REAC  78
48 CONTINUE                            REAC  79
L=0                                     REAC  80
GO TO 20                                REAC  81
50 RM=RM+ANUM(N,JJ)*ATOM(2,KK)         REAC  82
V(J)=ATOM(3,KK)                         REAC  83
DATA(J)=ANUM(N,JJ)                      REAC  84
100 CONTINUE                           REAC  85
C
C     ADD CONTRIBUTIONS TO WP(K), HPP(K), AM(K), BOP(I,K) AND RH(K)  REAC  86
C
101 PCWT=PECWT(N)                      REAC  87
IF(MOLES) PCWT=PCWT*RM                 REAC  88
WP(K)=WP(K) + PCWT                     REAC  89
EM = ENTH(N)                           REAC  90
IF(NAME(N,5).NE.1ZERO) HPP(K)=HPP(K)+EM *PCWT/(RM*R)    REAC  91
AM(K)=AM(K)+PCWT/RM                   REAC  92
DO 110 J=1,L                           REAC  93
BOP(J,K)=DATA(J)*PCWT/RM +BOP(J,K)  REAC  94
110 CONTINUE                           REAC  95
IF(DENS(N).NE.0.) GO TO 115           REAC  96
GO TO 117                                REAC  97
115 RH(K)=RH(K)+PCWT/DENS(N)          REAC  98
117 RMW(N) = RM                         REAC  99
N = N+1                                  REAC 100
IF(N.NE.16) GO TO 20                  REAC 101
200 NREAC =N-1                          REAC 102
IF(NFUEL.GT.0) GO TO 210               REAC 103
C
C     100 PERCENT OXIDANT, CALL REACTANTS FUEL                REAC 104
C
DC 205 N=1,NREAC                      REAC 105
FOX(N) = BLANK                         REAC 106
205 CONTINUE                           REAC 107
RH(2) = RH(1)                           REAC 108
RH(1) = 0.                               REAC 109
WF(2) = WP(1)                           REAC 110
WP(1) = 0.                               REAC 111
HPP(2) = HPP(1)                         REAC 112
AM(2) = AM(1)                           REAC 113
AM(1) = 0.                               REAC 114
DO 208 J=1,L                           REAC 115
BOP(J,2) = BOP(J,1)                     REAC 116
208 CCNTINUE                           REAC 117
210 IF(L.EQ.0) GO TO 1000               REAC 118
C
C     NORMALIZE HPP(K),AM(K),BOP(I,K), AND PECWT(N).        REAC 119
C     CALCULATE RH(K), V+(K), AND V-(K)                      REAC 120
C

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DC 220 K=1,2          REAC 127
IF (WP(K).EQ.0.) GO TO 220   REAC 128
HPP(K)=HPP(K)/WP(K)   REAC 129
AM(K) = WP(K)/AM(K)   REAC 130
IF (RH(K).NE.0.) RH(K)=WP(K)/RH(K)   REAC 131
DC 215 J=1,L          REAC 132
BOP(J,K)=BOP(J,K)/WP(K)   REAC 133
IF (V(J).LT.0.) VMIN(K)= VMIN(K)+BOP(J,K)*V(J)   REAC 134
IF (V(J).GT.0.) VPLS(K)=VPLS(K)+BOP(J,K)*V(J)   REAC 135
215 CONTINUE          REAC 136
IF (MOLES) GO TO 220   REAC 137
DO 218 N=1,NREAC      REAC 138
IF (FOX(N).EQ.OX.AND.K.EQ.2) GO TO 218   FEAC 139
IF (FOX(N).NE.OX.AND.K.EQ.1) GO TO 218   REAC 140
PECWT(N) = PECWT(N)/WP(K)   REAC 141
218 CONTINUE          REAC 142
220 CONTINUE          REAC 143
NEWR=.TRUE.           REAC 144
C ARE ELEMENTS SAME AS FOR LAST SET OF REACTANTS, IF SO, NEWR=.FALSE. REAC 145
C
IF (NLM.NE.NLS) GO TO 226   REAC 146
IF (NOMIT.NE.0) GO TO 226   REAC 147
DO 224 I=1,NLS          REAC 148
DO 222 J=1,NLM          REAC 149
IF (LLMT(J).NE.LLMTS(I)) GO TO 222   REAC 150
SBOP(I,1) = BOP(J,1)   REAC 151
SBOP(I,2) = BOP(J,2)   REAC 152
GO TO 224              REAC 153
222 CONTINUE          REAC 154
GO TO 226              REAC 155
224 CONTINUE          REAC 156
NEWR = .FALSE.          REAC 157
DO 225 I=1,NIM          REAC 158
LLMT(I) = LLMTS(I)      REAC 159
BOP(I,1) = SBOP(I,1)    REAC 160
BOP(I,2) = SBOP(I,2)    REAC 161
225 CCNTINUE          REAC 162
GO TO 229              REAC 163
C
C
226 NLS = NLM          REAC 164
NOMIT = 0               REAC 165
REWIND 4                REAC 166
DO 228 I=1,NLM          REAC 167
LLMITS(I) = LLMT(I)    REAC 168
228 CONTINUE          REAC 169
229 DC 230 N=1,NREAC    REAC 170
IF (DENS(N).NE.0.) GO TO 230   REAC 171
RH(2) = 0.               REAC 172
RH (1) = 0.               REAC 173
GO TO 1000              REAC 174
230 CONTINUE          REAC 175
1000 RETURN             REAC 176
END                     REAC 177
C
SUBROUTINE HCALC        HCAL  1
C
CALCULATE PROPERTIES FOR TOTAL REACTANT USING THERMO DATA FOR HCAL  2
C
HCAL  3

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C ONE OR MORE REACTANTS. HCAL 4
C DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS HCAL 5
C DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN HCAL 10
C LOGICAL MOLES,VOL,SHOCK,CALCH HCAL 11
C CALCULATE ENTHALPY FOR PROPELLANT USING COEFFICIENTS HCAL 12
C DIMENSION NUM(15,5) HCAL 13
C HCAL 14
C HCAL 15
C HCAL 16
C COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) HCAL 17
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) HCAL 18
2 ,VLM(13),TCTN(13) HCAL 19
COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250) MAIN 22
1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250) MAIN 23
COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) HCAL 22
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) HCAL 23
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5) HCAL 24
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) HCAL 25
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE HCAL 26
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM HCAL 27
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ HCAL 28
2 ,IONS,NC,INSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHHCAL 29
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM HCAL 30
C HCAL 31
EQUIVALENCE (ANUM,NUM),(L,NLM),(J,JS1) HCAL 32
EQUIVALENCE (AM1,DATA(20)),(CPR1,DATA(21)) HCAL 33
DATA AG/1HG/,IZERO/2H00/,OX/1H0/,BLK/1H / HCAL 34
C HCAL 35
KOD = 0 2/24/72
TSAVE = TT HCAL 36
C HCAL 37
C CALCUALTE MOLECULAR WEIGHT OF TOTAL REACTANT, AM1. HCAL 38
C HCAL 39
IF (AM(1).NE.0.0 .AND. AM(2).NE.0.0) GO TO4 HCAL 40
AM1= AM(2)
IF (AM(2).EQ.0.0) AM1= AM(1)
GC TO 9 HCAL 42
4 AM1=(CF+1.)*AM(1)*AM(2)/(AM(1)+OF*AM(2)) HCAL 43
9 TM = 0.
IF (PP.GT.0.) TM = ALOG (PP*AM1) HCAL 44
SSUM(NPT) = 0.
HPP(1) = 0.
HPP(2) = 0.
HSUB0 = 0.
CPR1 = 0.
ANN = (1.+OF) HCAL 45
C HCAL 53
C LOOP ON REACTANTS. HCAL 54
C IF OXIDANT, K=1 HCAL 55
C IF FUEL, K=2 HCAL 56
C HCAL 57
DO 900 N=1,NREAC HCAL 58
K=2
IF (FOX(N).EQ.OX) K=1 HCAL 59
IF (NAME(N,5).NE.IZERO) GO TO 89 HCAL 60
IF (.NOT.CALCH.AND.TT.NE.0.) GO TO 15 HCAL 61
TT = RTEMP(N) HCAL 62
C HCAL 63
C IS TT IN RANGE HCAL 64
HCAL 65

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C      15 IF(SHCCK) GO TO 16          HCAL 66
      IF(TT.LT.(TLLOW/1.2).OR.TT.GT.(THIGH*1.2)) GO TO 75  HCAL 67
      16 J = NUM(N,5)          HCAL 68
      IF (J.NE.0) GO TO 90          HCAL 69
      DO 10 J=1,L          HCAL 70
      DATA(J)=0.          HCAL 71
      10 CCNTINUE          HCAL 72
      HCAL 73
C      TEMPORARILY STORE STOICHIOMETRIC COEFFICIENTS IN DATA ARRAY.  HCAL 74
C
      DO 40 I=1,4          HCAL 75
      IF(ANUM(N,I).EQ.0.)GO TO 50  HCAL 76
      DO 20 J=1,L          HCAL 77
      IF(LLMT(J).EQ.NAME(N,I)) GO TO 30  HCAL 78
      20 CONTINUE          HCAL 79
      30 DATA(J)=ANUM(N,I)          HCAL 80
      40 CONTINUE          HCAL 81
      50 IS=0          HCAL 82
      HCAL 83
C      SEARCH FOR REACTANT IN THERMO SPECIES.  STORE INDEX IN NUM(N,5).  HCAL 84
C
      DC 70 J=1,NS          HCAL 85
      IF(IUSE(J).EQ.0)GO TO 55  HCAL 86
      IS = IS+1          HCAL 87
      IF(FAZ(N).EQ.AG)GO TO 70  HCAL 88
      IF(TT.GT.TEMP(IS,2).AND.TEMP(IS,2).NE.THIGH) GO TO 70  HCAL 89
      IF(TT.LT.TEMP(IS,1).AND.TEMP(IS,1).NE.TLOW) GO TO 70  HCAL 90
      GO TO 56          HCAL 91
      55 IF(FAZ(N).NE.AG.AND.FAZ(N).NE.BLK) GO TO 70  HCAL 92
      56 DO 60 I=1,L          HCAL 93
      IF(A(I,J).NE.DATA(I)) GO TO 70  HCAL 94
      60 CONTINUE          HCAL 95
      NUM(N,5) = J          HCAL 96
      GC TO 90          HCAL 97
      70 CONTINUE          HCAL 98
      GO TO 80          HCAL 99
      HCAL 100
C      CALCULATE EN FOR REACTANT AND CALL CPHS TO CALCULATE PROPERTIES.  HCAL 101
C
      89 KCD = 1          HCAL 102
      90 IF (MOLES)          ENJ = PECWT(N)/WP(K)          HCAL 103
      IF (.NOT.MOLES)          ENJ = PECWT(N)/RMW(N)          HCAL 104
      ENJ = ENJ/ANN          HCAL 105
      2/24/72
      IF(K.EQ.1) ENJ = ENJ*OF          HCAL 106
      IF(NAME(N,5).NE.IZERO)GO TO 500  HCAL 107
      NSS = NS          HCAL 108
      NS = NSS          HCAL 109
      NS = J          HCAL 110
      TLN = ALOG(TT)          HCAL 111
      IF(.NOT.CALCH) EN(J,NPT) = ENJ          HCAL 112
      CALL CPHS          HCAL 113
      NS = NSS          HCAL 114
      IF (HO(J).GT.-.01 .AND. HO(J).LT..01) HO(J) = 0.          HCAL 115
      RTEMP(N) = TT          HCAL 116
      IF(VOL) HO(J)=HO(J)-1.          HCAL 117
      ENTH(N) = HO(J)*R*TT          HCAL 118
      HCAL 119
C      ADD CONTRIBUTION TO CP, H, AND S OF TOTAL REACTANT.          HCAL 120
C
      HCAL 121
      HCAL 122
      HCAL 123

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CPR1 = CPR1 + CPSUM          HCAL 124
SSUM(NPT) = SSUM(NPT) + ENJ * (S(J)-ALOG(ENJ)-TM)  HCAL 125
500 ER = ENTH(N)*ENJ/R      HCAL 126
HSUB0 = HSUB0+ER           HCAL 127
HPP(K) = HPP(K)+ER         HCAL 128
900 CCNTINUE                HCAL 129
IF(TSAVE.NE.0.) TT=TSAVE    HCAL 130
GO TO 1000                  HCAL 131
75 WRITE(6,76)                HCAL 132
76 FORMAT(50H0REACTANT TEMPERATURE OUT OF RANGE OF THERMO DATA )  HCAL 133
TT = 0.                      HCAL 134
GO TO 1000                  HCAL 135
80 WRITE(6,85) N             HCAL 136
85 FORMAT(9H0REACTANT,I2,22H IS NOT IN THERMO DATA )  HCAL 137
TT = 0.                      HCAL 138
1000 IF (KOD.EQ.1) CPR1 = 0. 2/24/72
      RETURN
      END
      SUBROUTINE SAVE          HCAL 140
C
C   SAVES OR USES COMPOSITIONS FROM PREVIOUS POINT AS INITIAL ESTIMATES  SAVE 3
      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN          SAVE 9
C
C   LOGICAL VOL,CALCH,IONS,SHOCK                         SAVE 10
C
C   COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250)  MAIN 22
      1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250)  MAIN 23
      COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)  SAVE 15
      1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)  SAVE 16
      2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        SAVE 17
      3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)  SAVE 18
      4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE,SIZE       SAVE 19
      COMMON/INDX/ IDEBUG,CONVG,TF,HP,SP,ISV, NPP, MOLES, NP, NT, NPT, NLM  SAVE 20
      1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ  SAVE 21
      2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHSAVE 22
      3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM                     SAVE 23
C
C   EQUIVALENCE (AC(1),JSOLS),(AC(2),JLIQS)            SAVE 24
C
C   DATA IE/1HE/                                     SAVE 25
      IF(ISV) 100,10,200                            SAVE 26
C
C   NEXT POINT FIRST T IN SCHEDULE, USE PREVIOUS COMPOSITIONS FOR THIS T  SAVE 31
C
10 IQ1 = IQSAVE                SAVE 32
JSOL = JSOLS                  SAVE 33
JLIQ = JLIQS                  SAVE 34
ENN = ENSAVE                  SAVE 35
ENNL = ENLSAV                 SAVE 36
NLM = LSAVE                   SAVE 37
DC 50 J = 1,NS                 SAVE 38
IF (IUSE(J).EQ.0) GO TO 20     SAVE 39
EN (J,NPT) = SLN(J)           SAVE 51
IF(IUSE(J).GT.0) IUSE(J) = - IUSE(J)  SAVE 52
IF (EN(J,NPT).NE.0.) IUSE(J) = -IUSE(J)  SAVE 53
GO TO 50                       SAVE 54
20 EN(J,NPT) = 0.              SAVE 55
ENLN(J) = SLN(J)               SAVE 56
                                SAVE 57

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IF(SLN(J).EQ.0.) GO TO 50
IF ((ENLN(J)-ENN + 18.5).LE.0.) GO TO 50
EN(J,NPT) = 2.718281828459**ENLN(J)
50 CONTINUE
GO TO 1000

C FIRST T--SAVE COMPOSITIONS FOR FUTURE POINTS WITH THIS T
C
100 ISV = -ISV
JSOLS = JSOL
JLIQS = JLIQ
IQSAVE = IQ1
ENSAVE = ENN
ENLSAV = ENNL
LSAVE = NLM
DO 150 J = 1,NS
SIN(J) = ENLN(J)
IF(IUSE(J).NE.0) SLN(J)=EN(J,ISV)
150 CCNTINUE

C USE COMPOSITIONS FROM PREVIOUS POINT
C
200 DC 300 J = 1,NS
EN(J,NPT) = EN(J,ISV)
300 CONTINUE
1000 RETURN

C CALCULATE NEW VALUES OF BO AND HSUB0 FOR NEW OF RATIO
C
ENTRY NEWOF

C
C WRITE(6,730) OF
730 FORMAT(6H0OF = ,F10.6)
EQRAT = 0.
SUM = OF + 1.
V2 = (OF*VMIN(1)+VMIN(2))/SUM
V1 = (OF*VPLS(1)+VPLS(2))/SUM
IF(V2.NE.0.) EQRAT=ABS(V1/V2)
IF (RH(1) .NE. 0. .AND. RH(2) .NE. 0.) GO TO 744
RHOP = RH(2)
IF (RHOP .EQ. 0.) RHOP = RH(1)
GO TO 745
744 RHOP = (OF+1.)*RH(1)*RH(2)/(RH(1) + OF *RH(2))
745 DO 747 I=1,NLM
BO(I) = (OF *BOP(I,1)+ BOP(I,2))/SUM
IF(I.NE.1) GO TO 746
BIGB = BO(1)
SMALB = BO(1)
GO TO 747
746 IF(BO(I).EQ.0.) GO TO 747
IF(BO(I).LT.SMALB) SMALB=BO(I)
IF(BO(I).GT.BIGB) BIGB=BO(I)
747 CONTINUE
NPT = 1
IF(.NOT.CALCH) GO TO 750
CALL HCALC
IF(TT.EQ.0.) RETURN
CALCH = .FALSE.

SAVE 58
SAVE 59
SAVE 60
SAVE 62
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SAVE 93
SAVE 94
SAVE 95
SAVE 96
SAVE 97
SAVE 98
SAVE 99
SAVE 100
SAVE0101
SAVE0102
SAVE0103
SAVE0104
SAVE0105
SAVE0106
SAVE0107
SAVE0108
SAVE0109

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IF (OF.NE.0.) HPP(1)=SUM*HPP(1)/OF          SAVE0110
HPP(2) = SUM*HPP(2)                         SAVE0111
GO TO 760                                     SAVE0112
750 HSUB0= (OF*HPP(1) + HPP(2))/SUM          SAVE0113
760 IC = 0                                     SAVE0114
      TEM = SMALB/BIGB
      SIZE = 18.420681
      IF (TEM.LT.1.E-5) SIZE=ALOG(1000./TEM)    SAVE0115
      JSOL = 0
      JLIQ = 0
      WRITE (6,770)
770 FORMAT(1H ,25X,14HEFFECTIVE FUEL,10X,17HEFFECTIVE OXIDANT,12X,7HMISAVE0118
1XTURE )
      IF (VOL) WRITE(6,772)                      SAVE0119
      IF (.NOT.VOL) WRITE(6,774)                  SAVE0120
772 FORMAT(16H INTERNAL ENERGY,14X,6HHPP(2),19X,6HHPP(1),19X,5HHSUB0 )SAVE0122
774 FORMAT(9H ENTHALPY,21X,6HHPP(2),19X,6HHPP(1),19X,5HHSUB0 )SAVE0123
      WRITE(6,776)HPP(2),HPP(1),HSUB0           SAVE0124
776 FORMAT(19H (KG-MOL) (DEG K)/KG,E21.8,2E25.8 )SAVE0125
      WRITE(6,778)
778 FORMAT(12HOKG-ATOMS/KG,17X,8HBOP(I,2),17X,8HBOP(I,1),18X,5HB0(I))SAVE0127
780 FCRRMAT(8X,A2,5X,3E25.8)
      WRITE(6,780)(LLMT(I),           BOP(I,2),BOP(I,1),B0(I),I=1,NLM)SAVE0128
      RETURN
      END

```

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C
C
      SUBROUTINE CPHS                         CPHS   1
C      CALCULATES THERMODYNAMIC PROPERTIES FOR INDIVIDUAL SPECIES  CPHS   2
C
C      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN                         CPHS   6
C
C      COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250)  CPHS   8
C      1,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250)  CPHS   9
C      COMMON/MISC/ENN,SUMN,TT,S0,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) CPHS  12
C      1,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)CPHS 13
C      2,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)        CPHS  14
C      3,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)CPHS 15
C      4,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE          CPHS  16
C      COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NFT,NLM CPHS  17
C      1,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ CPHS  18
C      2,ICNS,NC,INSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHCPHS 19
C      3,IQSAVE,LSAVE,ISUP,ISUB,ITNUM                           CPHS  20
C
C      EQUIVALENCE (J,JS1)                         CPHS  21
C
C      K = 1                                         CPHS  22
C      IF (TT.LE.TMID)K = 2                         CPHS  23
C      KK = 0                                         CPHS  24
C      CPSUM=0.                                       CPHS  25
C
C      90 IF(COEF(K,1,J).NE.0.)GO TO 97            CPHS  26
C      IF (IUSE(J).LT.0) GO TO 100                 CPHS  27
C
C      IF COEFFICIENTS ARE ZERO, USE OTHER TEMPERATURE INTERVAL CPHS  28
C
C      KK = K                                         CPHS  29
C      K = 1                                         CPHS  30
C      IF (KK.EQ.1) K = 2                         CPHS  31
C
C

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97 S(J) = (((((COEF(K,5,J)/4.)*TT+ COEF(K,4,J)/3.)*TT+ COEF(K,3,J)/2.CPHS 36
1)* TT+COEF(K,2,J))*TT+ COEF(K,1,J)*TLN + COEF(K,7,J) CPHS 37
H0(J) = (((((COEF(K,5,J)/5.)*TT+ COEF(K,4,J)/4.)*TT+ COEF(K,3,J)/3.CPHS 38
1 ) *TT+ COEF(K,2,J)/2.)*TT+ COEF(K,1,J) + COEF(K,6,J)/TT CPHS 39
CPSUM= CPSUM+(((COEF(K,5,J)*TT+ COEF(K,4,J))*TT+ COEF(K,3,J))*TT CPHS 40
1 + COEF(K,2,J))*TT+ COEF(K,1,J))*EN(J,NPT) CPHS 41
IF (KK.EQ.0) GO TO 100 CPHS 42
KK = KK CPHS 43
KK = 0 CPHS 44
100 IF (J.EQ.NS) GO TO 200 CPHS 45
J=J+1 CPHS 46
GO TO 90 CPHS 47
200 RETURN CPHS 48
END CPHS 49
SUBROUTINE MATRIX MATX 1
C
C
C DOUBLE PRECISION G,X MATX 2
LOGICAL HP,SP,TP,IDEBUG,CONVG,NEWR,VOL,UV,SV,TV,LOGV MATX 3
C
C DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS MATX 4
DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN MATX 5
DOUBLE PRECISION H,F,SS,TERM1,TERM,SSS MATX 9
DOUBLE PRECISION EN1,EN2,SUMI,RAT1,RAT2 SOLN
DOUBLE PRECISION EN10,EN20,C1,C2 SOLN
C
COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) MATX 13
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) MATX 14
2 ,VLM(13),TOTN(13) MATX 15
COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250) MAIN 22
1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250) MAIN 23
COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) MATX 19
1 ,TM,TLCW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) MATX 20
2 ,HFP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5) MATX 21
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) MATX 22
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE MATX 23
COMMON /DOUBLE/ G(20,21), X(20) MATX 24
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM MATX 25
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ MATX 26
2 ,IONS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHMATX 27
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM MATX 28
CCMON/IS/JSOL1,JSOL2 SOLN
COMMON/COMP/EN10,EN20,C1,C2 SOLN
C
EQUIVALENCE (NLM,L),(TP,TV),(SV,SP),(UV,HP),(CPCVEQ,LOGV) MATX 29
C
C
IQ2 = IQ1 + 1 MATX 30
IQ3 = IQ2 + 1 MATX 31
KMAT = IQ3 MATX 32
IF(.NOT.CONVG.AND.TP) KMAT = IQ2 MATX 33
IMAT = KMAT - 1 MATX 34
C
CLEAR MATRIX STORAGES TO ZERO MATX 35
C
DO 211 I=1,IMAT MATX 36
DO 211 K=1,KMAT MATX 37
G(I,K)= 0.0D0 MATX 38
211 CCNTINUE MATX 39
G (IQ2,IQ1) = 0. MATX 40

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SSS = 0.                                MATX 44
HSUM(NPT) = 0.                            MATX 45
C
C BEGIN SET UP OF ITERATION MATRIX        MATX 46
C
KK = L
DO 65 J=1,NS
IF(IUSE(J).LT.0) GO TO 65
H=HO(J)*EN(J,NPT)
IF(IUSE(J).GT.0.AND.IUSE(J).LT.999) GO TO 70
IF(IUSE(J).EQ.999) GO TO 65
F = (HO(J)-S(J)+ENLN(J)+TM)*EN(J,NPT)
SS = H-F
TERM1 = H
IF (KMAT .EQ. IQ2) TERM1 = F
DO 55 I = 1, L
C
C CALCULATE THE ELEMENTS R(I,K)          MATX 54
C
IF (A(I,J) .EQ. 0.) GO TO 55
TERM= A(I,J)*EN(J,NPT)
DO 15 K=I, L
G(I,K)= G(I,K) + A(K,J)*TERM
15 CCNTINUE
C
G(I,IQ1)=G(I,IQ1)+TERM
G(I,IQ2)=G(I,IQ2)+A(I,J)*TERM1
IF (CONVG .OR.TP) GO TO 55
G(I,IQ3)= G(I,IQ3)+A(I,J)*F
IF (SF) G(IQ2,I) = G(IQ2,I) + A(I,J)*SS
55 CONTINUE
IF (KMAT .EQ. IQ2) GO TO 64
IF(CONVG.OR.HP) GO TO 59
G(IQ2,IQ1) = G(IQ2,IQ1) + SS
G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*SS
G(IQ2,IQ3) = G(IQ2,IQ3)+(S(J) - ENLN(J)-TM)*F
GC TO 62
59 G(IQ2,IQ2)=G(IQ2,IQ2)+HO(J)*H
IF (CONVG) GO TO 64
G(IQ2,IQ3)=G(IQ2,IQ3)+HO(J)*F
62 G(IQ1,IQ3)=G(IQ1,IQ3)+F
64 G(IQ1,IQ2)=G(IQ1,IQ2)+TERM1
GO TO 65
C
C CONDENSED SPECIES                      MATX 55
C
70 KK = KK + 1
DO 75 I = 1, L
G(I,KK) = A(I,J)
G(I,KMAT) = G(I,KMAT) - A(I,J)*EN(J,NPT)
75 CONTINUE
G(KK,IQ2) = HO(J)
G(KK,KMAT) = HO(J) - S(J)
HSUM(NPT) = HSUM(NPT) + H
IF(.NOT.SP) GC TO 65
SSS = SSS + S(J)*EN(J,NPT)
G(IQ2,KK) = S(J)
65 CONTINUE
SSS = SSS + G(IQ2,IQ1)

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HSUM(NPT) = HSUM(NPT) + G(IQ1,IQ2)          MATX 102
G(IQ1,IQ1) = SUMN - ENN                      MATX 103
C
C      REFLECT SYMMETRIC PORTIONS OF THE MATRIX    MATX 104
C
ISYM = IQ1                                     MATX 105
IF(HP.OR.CONVG) ISYM=IQ2                      MATX 106
DO 102 I=1,ISYM                                MATX 107
DC 102 J=I,ISYM                                MATX 108
G(J,I)=G(I,J)                                  MATX 109
102 CONTINUE                                     MATX 110
IF(IS.EQ.0) GOTO300                            MATX 111
KK1 = KK+1                                      MATX 112
KK2 = KK+2                                      SOLN
EN1 = EN(JSOL1,NPT)                            SOLN
EN2 = EN(JSOL2,NPT)                            SOLN
DO 310 I=1,L                                    SOLN
G(I,KMAT) = G(I,KMAT)-A(I,JSOL1)*EN1-A(I,JSOL2)*EN2
G(KK1,I) = A(I,JSOL1)                          SOLN
G(KK2,I) = A(I,JSOL2)                          SOLN
G(I,KK1) = A(I,JSOL1)                          SOLN
310 G(I,KK2) = A(I,JSOL2)                      SOLN
SUMI = 1.D0/(C1*EN1+C2*EN2)                    SOLN
RAT1 = C1*EN1*SUMI                            SOLN
RAT2 = C2*EN2*SUMI                            SOLN
G(KK1,KK1) = -C1*RAT2/EN1                     SOLN
G(KK1,KK2) = C1*C2*SUMI                      SOLN
G(KK2,KK1) = G(KK1,KK2)                      SOLN
G(KK2,KK2) = -C2*RAT1/EN2                     SOLN
G(KK1,KMAT) = HO(JSOL1)-S(JSOL1)+C1*DLOG(RAT1)
G(KK2,KMAT) = HO(JSOL2)-S(JSOL2)+C2*DLOG(RAT2)
300 CONTINUE                                     SOLN
C
C      COMPLETE THE RIGHT HAND SIDE               MATX 113
C
IF(.NOT.CONVG) GO TO 140                      MATX 114
IF(.NOT.LOGV) GO TO 175                      MATX 115
C
LOGV = .TRUE.-- SET UP MATRIX TO SOLVE FOR DLVPT   MATX 116
C
G(IQ1,IQ2) = ENN                           MATX 117
IQ = IQ1 - 1                                 MATX 118
DO 135 I = 1,IQ                           MATX 119
G(I,IQ2) = G(I,IQ1)                         MATX 120
135 CONTINUE                                     MATX 121
GO TO 175                                     MATX 122
140 DO 145 I=1,L                           MATX 123
X(1)=B0(I)-G(I,IQ1)                         MATX 124
G(I,KMAT) = G(I,KMAT)+X(1)                   MATX 125
145 CONTINUE                                     MATX 126
G(IQ1,KMAT) = G(IQ1,KMAT)+ENN-SUMN          MATX 127
C
C      COMPLETE ENERGY ROW AND TEMPERATURE COLUMN  MATX 128
C
IF (KMAT .EQ. IQ2) GO TO 185                MATX 129
IF (SP) ENERGY = S0+ENN-SUMN - SSS          MATX 130
IF(HP) ENERGY=HSUB0/TT - HSUM(NPT)          MATX 131
G(IQ2,IQ3)=G(IQ2,IQ3) + ENERGY             MATX 132
G(IQ2,IQ2) = G(IQ2,IQ2)+CPSUM             MATX 133
175

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185 IF(.NOT.VOL.OR.CONVG) GO TO 1000          MATX 140
C
C      CONSTANT VOLUME MATRIX                  MATX 141
C
C      IQ =IQ1-1                                MATX 142
C      IF(KMAT.EQ.IQ2) GO TO 230                MATX 143
C      DO 220 I=1,IQ                            MATX 144
C          G(IQ1,I) = G(IQ2,I)-G(IQ1,I)          MATX 145
C          G(I,IQ1) = G(I,IQ2)-G(I,IQ1)          MATX 146
C          G(I,IQ2) = G(I,IQ3)                   MATX 147
C 220 CONTINUE                                 MATX 148
C          G(IQ1,IQ1) = G(IQ2,IQ2)-G(IQ1,IQ2)-G(IQ2,IQ1)  MATX 149
C          G(IQ1,IQ2) = G(IQ2,IQ3)-G(IQ1,IQ3)  MATX 150
C          IF (UV) G(IQ1,IQ2) = G(IQ1,IQ2) + ENN   MATX 151
C          GO TO 260                            MATX 152
C 230 DO 240 I=1,IQ                            MATX 153
C          G(I,IQ1) = G(I,IQ2)                   MATX 154
C 240 CONTINUE                                 MATX 155
C 260 KMAT = IMAT                           MATX 156
C          IMAT = IMAT-1                      MATX 157
C 1000 RETURN                                  MATX 158
C          END
C          SUBROUTINE GAUSS                     MATX 159
C
C          SOLVE ANY LINEAR SET OF UP TO 20 EQUATIONS    GAUS 1
C          NUMBER OF EQUATIONS = IMAT                    GAUS 2
C
C          DOUBLE PRECISION G,X,COEFX(20),SUM,Z           GAUS 3
C
C          COMMON/DDOUBLE/G(20,21),X(20)                 GAUS 4
C          COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES, NP, NT, NPT, NLM  GAUS 5
C          1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ  GAUS 6
C          2 ,IONS,NC,INSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHGAUS 10
C          3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM               GAUS 11
C
C          DATA BIGNO/1.E+38/                         GAUS 12
C
C          BEGIN ELIMINATION OF NNTH VARIABLE        GAUS 13
C
C          IUSE1 = IMAT+1                           GAUS 14
C 6 DO 45  NN=1,IMAT                         GAUS 15
C          IF(NN-IMAT) 8,83,8                      GAUS 16
C 83 IF(G(NN,NN)) 31,23,31                  GAUS 17
C
C          SEARCH FOR MAXIMUM COEFFICIENT IN EACH ROW  GAUS 18
C
C 8 DO 18  I=NN,IMAT                         GAUS 19
C          CCEFX(I) = BIGNO                      GAUS 20
C          IF(G(I,NN).EQ.0.)  GO TO 18            GAUS 21
C          COEFX(I) = 0.                          GAUS 22
C          DO 10 J=NN,IUSE1                      GAUS 23
C          SUM = G(I,J)                         GAUS 24
C          IF(SUM.LT.0.)  SUM=-SUM              GAUS 25
C          IF(J.NE.NN)  GO TO 9                GAUS 26
C          Z = SUM                           GAUS 27
C          GO TO 10                         GAUS 28
C 9 IF(SUM.GT.COEFX(I))  COEFX(I)=SUM       GAUS 29
C 10 CONTINUE                                 GAUS 30
C          CCEFX(I) = COEFX(I)/Z             GAUS 31

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18	CONTINUE	GAUS	38
		GAUS	39
	LOCATE ROW WITH SMALLEST MAXIMUM COEFFICIENT	GAUS	40
	TEMP = BIGNO	GAUS	41
	I=0	GAUS	42
20	DO 22 J=NN,IMAT	GAUS	43
	IF (COEFX(J)-TEMP) 87,22,22	GAUS	44
87	TEMP=COEFX(J)	GAUS	45
	I=J	GAUS	46
22	CONTINUE	GAUS	47
	IF(I) 28,23,28	GAUS	48
	INDEX I LOCATES EQUATION TO BE USED FOR ELIMINATING THE NTH	GAUS	49
	VARIABLE FROM THE REMAINING EQUATIONS	GAUS	50
	INTERCHANGE EQUATIONS I AND NN	GAUS	51
28	IF(NN-I) 29,31,29	GAUS	52
29	DC 30 J=NN,IUSE1	GAUS	53
	Z=G(I,J)	GAUS	54
	G(I,J)=G(NN,J)	GAUS	55
	G(NN,J)=Z	GAUS	56
30	CONTINUE	GAUS	57
	DIVIDE NTH ROW BY NTH DIAGONAL ELEMENT AND ELIMINATE THE NTH	GAUS	58
	VARIABLE FROM THE REMAINING EQUATIONS	GAUS	59
31	K = NN + 1	GAUS	60
	DO 36 J = K, IUSE1	GAUS	61
	IF(G(NN,NN).EQ.0.) GO TO 23	GAUS	62
	G(NN,J) = G(NN,J) / G(NN,NN)	GAUS	63
36	CONTINUE	GAUS	64
	IF(K-IUSE1) 86,45,88	GAUS	65
88	DO 44 I=K,IMAT	GAUS	66
40	DO 44 J = K, IUSE1	GAUS	67
	G(I,J) = G(I,J) - G(I,NN)*G(NN,J)	GAUS	68
44	CONTINUE	GAUS	69
45	CONTINUE	GAUS	70
	BACKSOLVE FOR THE VARIABLES	GAUS	71
	K = IMAT	GAUS	72
47	J = K + 1	GAUS	73
	X(K) = 0.0D0	GAUS	74
	SUM = 0.0	GAUS	75
	IF(IMAT-J) 51,48,48	GAUS	76
48	DO 50 I=J,IMAT	GAUS	77
	SUM = SUM + G(K,I)* X(I)	GAUS	78
50	CONTINUE	GAUS	79
51	X(K) = G(K,IUSE1) - SUM	GAUS	80
	K = K - 1	GAUS	81
	IF (K) 47,151,47	GAUS	82
23	IMAT = IMAT-1	GAUS	83
151	RETURN	GAUS	84
	END	GAUS	85
	SUBROUTINE VARFMT(V,NPT)	VRFT	86
	DIMENSION V(13)	VRFT	87
		VRFT	88
		VRFT	89
		VRFT	90
		VRFT	91
		VRFT	92
		VRFT	93
		VRFT	1
		VRFT	2
		VRFT	3

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C      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)    VRFT   4
1      ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2    VRFT   5
2      ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO    VRFT   6
C      DO 45 I=1,NPT    VRFT   7
      K= 2*I+3    VRFT   8
      FMT(K) = F4    VRFT   9
      IF (V(I).GE.10.) FMT(K) = F3    VRFT  10
      IF (V(I).GE.100.) FMT(K) = F2    VRFT  11
      IF (V(I).GE.10000.) FMT(K) = F1    VRFT  12
      IF (V(I).GE.1000000.) FMT(K) = F0    VRFT  13
45     CONTINUE    VRFT  14
      RETURN    VRFT  15
      END    VRFT  16
      SUBROUTINE EFMT(NPT,AA,V)    EFMT   1
C      DIMENSION AA(3), V(13), W(13), NE(13), FRMT(7)    EFMT   2
C      COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)    EFMT   3
1      ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2    EFMT   4
2      ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO    EFMT   5
C      DATA FRMT/3H(1H,4H,3A4,4H,11X,4H,13(,4HF7.4,4H,I2),1H)/,F63/4HF6.3EFMT   6
1/,FI3/4H,I3)/,F74/4HF7.4/,FI2/4H,I2)/,F11X/4H,11X/,F2X/3H,2X/    EFMT   7
C      THE FOLLOWING DOUBLE PRECISION TYPE STATEMENTS ARE REQUIRED FOR    DETN   8
      FRMT(5) = F74    EFMT  11
      FRMT(6) = FI2    EFMT  12
      J1 = 1    EFMT  13
      FRMT(3) = F2X    EFMT  14
      IF(FMT(4).NE.FMT9X) GO TO 130    EFMT  15
      J1 = 2    EFMT  16
      FRMT(3) = F11X    EFMT  17
130    DO 145 I=J1,NPT    EFMT  18
      IF(V(I).NE.0.) GO TO 140    EFMT  19
      W(I) = 0.    EFMT  20
      NE(I) = 0.    EFMT  21
      GO TO 145    EFMT  22
      140 EE = ALOG10(ABS(V(I)))    EFMT  23
      NE(I) = EE    EFMT  24
      FE = NE(I)    EFMT  25
      IF(EE.LE.0..AND.FE.NE.EE) NE(I)=NE(I)-1    EFMT  26
      IF(IABS(NE(I)).LT.10) GO TO 144    EFMT  27
      FRMT(5) = F63    EFMT  28
      FRMT(6) = FI3    EFMT  29
      144 W(I) = V(I)/10.**NE(I)    EFMT  30
      145 CONTINUE    EFMT  31
      WRITE(6,FRMT) (AA(I),I=1,3),(W(J),NE(J),J=J1,NPT)    EFMT  32
1000   RETURN    EFMT  33
      END    EFMT  34
      SUBROUTINE OUT1    EFMT  35
C      DOUBLE PRECISION G,X    OUTP   1
      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS    OUTP   2
      DOUBLE PRECISION COEFF,S,EN,ENLN,HO,DELN    OUTP   3
C      LOGICAL EQL,FROZ,TP,HP,SP,HPSP,TPSP,MCLES,VOL    OUTP   8
C                                         OUTP   9
C                                         OUTP  10
C                                         OUTP  11
C                                         OUTP  12

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C DIMENSION NV(13),Z(10,3),HEAD(15),YX(5),YN(5),FSB(3),FRHO(3) OUTP 13
C CCOMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13) OUTP 14
C 1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13) OUTP 15
C 2 ,VLM(13),TOTN(13) OUTP 16
C CCOMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250) MAIN 22
C 1 ,DEIN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250) MAIN 23
C COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2) OUTP 20
C 1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2) OUTP 21
C 2 ,HPP(2),RH(2), VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5) OUTP 22
C 3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15) OUTP 23
C 4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENN,ENSAVE,ENLSAV,TRACE OUTP 24
C COMMON /DOUBLE/ G(20,21), X(20) OUTP 25
C COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM OUTP 26
C 1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ OUTP 27
C 2 ,IONS,NC,NSEPT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCHOUTP 28
C 3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM OUTP 29
C COMMON/PERF/PCP(22),VMOC(13),SPIM(13),VACI(13),SUBAR(13),SUPAR(13) OUTP 30
C 1 ,APP(13),AEAT(13),CSTR,EQL,FROZ,SS0,AREA,AWT OUTP 31
C COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4) OUTP 32
C 1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2 OUTP 33
C 2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO OUTP 34
C OUTP 35
C EQUIVALENCE (V,NV),(Z,H0),(IB,FB) OUTP 36
C OUTP 37
C HEAD=(1H ,2A4.5 (A2,F8.5,3X),5 X,F7.5,F13.3,4X,A1,F10.2,F9.4) OUTP 38
C OUTP 39
C DATA HEAD/4H(1H ,4H,2A4,2H,5,4H(A2,,4HF8.5 ,4H,3X),2H,5 ,2HX, OUTP 40
C 1 ,4HF7.5 ,4H,F13 ,4H.3,4 ,4HX,A1 ,4H,F10 ,4H.2,F ,4H9.4)/ OUTP 41
C DATA FUEL/4HFUEL/,OXID/4HOXID/,ANT/3HANT/,OX/1HO/,IZ/2H00/ OUTP 42
C 1 ,YN/2H,1, 2H,2, 2H,3, 2H,4, 2H,5 /,F75/4HF7.5/ OUTP 43
C 2 ,YX/3H,57,3H,44,3H,31,3H,18,2H,5 /,F73/4HF7.3/ OUTP 44
C DATA FRHO/4HRHO,,4H G/C,1HC/ OUTP 45
C
C IF(KASE.NE.0) WRITE (6,3) KASE OUTP 47
C 3 FORMAT (9H CASE NO. ,1B) OUTP 48
C IF(.NOT.MOLES) WRITE(6,5) OUTP 49
C 5 FORMAT (77X,46HWT FRACTION ENERGY STATE TEMP DENSITY/ OUTP 50
C 1 10X,16HCHEMICAL FORMULA,51X,21H(SEE NOTE) CAL/MOL,10X,5HDEG K,OUTP 51
C 2 4X,4HG/CC ) OUTP 52
C IF(MOLES) WRITE(6,6) OUTP 53
C 6 FORMAT (79X,5HMOLES,7X, 33H ENERGY STATE TEMP DENSITY/ OUTP 54
C 1 10X,16HCHEMICAL FORMULA,66X,7HCAL/MOL,10X,13HDEG K G/CC ) OUTP 55
C DO 15 N=1,NREAC OUTP 56
C IF(FOX(N).NE.OX) GO TO 10 OUTP 57
C HD1 = OXID OUTP 58
C HD2 = ANT OUTP 59
C GO TO 11 OUTP 60
C 10 HD1 = FUEL OUTP 61
C HD2 = FB OUTP 62
C 11 DO 13 J=1,5 OUTP 63
C IF(NAME(N,J).EQ.IZ.OR.NAME(N,J).EQ.IB) GO TO 14 OUTP 64
C 13 CCNTINUE OUTP 65
C J=6 OUTP 66
C 14 J=J-1 OUTP 67
C HEAD(3)=YN(J) OUTP 68
C HEAD(7)=YX(J) OUTP 69
C HEAD(9) = F75 OUTP 70
C IF(PECWT(N).GE.10.) HEAD(9)=F73 OUTP 71

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      WRITE(6,HEAD) HD1,HD2,(NAME(N,JJ),ANUM(N,JJ),JJ=1,J),PECWT(N),ENTH(OUTP 72
      1N), FAZ(N),RTEMP(N),DENS(N)
15 CONTINUE
      FPC = 100./ (1.+OF)
      WRITE(6,20) OF ,FPC,EQRAT,RHOP
20 FORMAT (1H0,15X,4H0/F=,F8.4,4X,13HPERCENT FUEL=,F8.4,4X,
1 19HEQUIVALENCE RATIO= ,F7.4,4X,17HREACTANT DENSITY=,F8.4//)
C      OUTP 73
C      OUTP 74
C      OUTP 75
C      OUTP 76
C      OUTP 77
C      OUTP 78
C      OUTP 79
C      OUTP 80
C      OUTP 81
C      OUTP 82
C      OUTP 83
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C      OUTP 123
C      OUTP 124
C      OUTP 125
C      OUTP 126
C      OUTP 127
C      OUTP 128
C      OUTP 129
C      OUTP 130
C      OUTP 131
C      OUTP 132
C      OUTP 133
C      OUTP 134
C      OUTP 135

      AGV = 9.80665
      RETURN

C      ENTRY OUT2
      FMT(4) = FMT(6)

C      PRESSURE
C      CALL EFMT(NET,FP,PPP)

C      TEMPERATURE
C      DO 64 65 I=1,NPT
      NV(I) = TTT(I)+.5
65 CONTINUE
      FMT(4) = FMT13
      FMT(5) = FMTI9
      WRITE (6,FMT)(FT(I),I=1,4),(NV(J),J=1,NPT)

C      DENSITY
C      DO 70 71 I=1,NPT
      IF(VLM(I).NE.0.) V(I)=1./VLM(I)
70 CONTINUE
      CALL EFMT(NPT,FRHO,V)

C      ENTHALPY
C      DC 75 I=1,NPT
      V(I) = HSUM(I) * R
75 CONTINUE
      FMT(5) = FB
      IF(R.LT.10.) GO TO 76
      CALL EFMT(NPT,FH,V)
      FMT(7) = F1
      GO TO 77
76 FMT(7) = F1
      WRITE (6,FMT)(FH(I),I=1,4),(V(J),J=1,NPT)

C      ENTROPY
      FMT(7)=F4
77 DO 78 I=1,NPT
      V(I) = SSUM(I) * R
78 CONTINUE
      WRITE (6,FMT)(FS(I),I=1,4),(V(J),J=1,NPT)
      WRITE (6,80)
80 FCRRMAT ( 1H )

C      MOLECULAR WEIGHT
      FMT(7) = F3

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      WRITE (6,FMT) (FM(I),I=1,4), (WM(J),J=1,NPT)          OUTP 136
C      (DLV/DLP) T                                         OUTP 137
C
C      FMT(7)=F5                                         OUTP 138
C      IF(EQL)  WRITE(6,FMT) (FV(I),I=1,4), (DLVPT(J),J=1,NPT) OUTP 139
C
C      (DLV/DLT) P                                         OUTP 140
C
C      FMT(7)= F4                                         OUTP 141
C      IF(EQL)  WRITE(6,FMT) (FD(I),I=1,4), (DLVTP(J),J=1,NPT) OUTP 142
C
C      HEAT CAPACITY                                     OUTP 143
C
C      IF(R.GT.10.) FMT(7)=F1                           OUTP 144
C      DO 85 I=1,NPT                                    OUTP 145
C      V(I) = CPR(I) * R                            OUTP 146
85 CONTINUE                                         OUTP 147
      WRITE(6,FMT) (FC(I),I=1,4), (V(J),J=1,NPT)          OUTP 148
C
C      GAMMA(S)                                         OUTP 149
C
C      FMT(7) = F4                                       OUTP 150
C      WRITE(6,FMT) (FG(I),I=1,4), (GAMMAS(J),J=1,NPT)    OUTP 151
C
C      SONIC VELOCITY                                  OUTP 152
C
C      FMT(7)= F1                                       OUTP 153
C      DO 95 I = 1,NPT                                 OUTP 154
C      SONVEL(I) = (RR*GAMMAS(I)*TTT(I)/WM(I))**.5   OUTP 155
95 CONTINUE                                         OUTP 156
      WRITE(6,FMT) (FL(I),I=1,4), (SONVEL(J),J=1,NPT)    OUTP 157
      RETURN                                            OUTP 158
C
C      ENTRY CUT3                                      OUTP 159
C
C      TRA = 5.E-6                                     OUTP 160
C      IF(TRACE.NE.0.) TRA= TRACE                     OUTP 161
C      IF(.NOT.EQL) GO TO 331                         OUTP 162
C
C      MOLE FRACTIONS - EQUILIBRIUM                  OUTP 163
C
C      WRITE (6,80)                                     OUTP 164
C      FMT(7)= F5                                       OUTP 165
C      WRITE(6,310)                                     OUTP 166
C
310 FORMAT(15H MOLE FRACTIONS //)                   OUTP 167
      DO 316 I=1,NPT                                 OUTP 168
      IF(TRACE.EQ.0.) GO TO 317                      OUTP 169
      IF(V(I).GE.TRACE) GO TO 325                  OUTP 170
317 IF(V(I).GE.(5.E-6)) GO TO 320                OUTP 171
316 CONTINUE                                         OUTP 172
      GO TO 330                                         OUTP 173
320 WRITE (6,FMT) SUB(K,1),SUB(K,2),SUB(K,3),FB,(V(I),I=1,NPT) OUTP 174
      GO TO 330                                         OUTP 175
325 FSB(1) = SUB(K,1)                             OUTP 176
      FSB(2) = SUB(K,2)                             OUTP 177
      FSB(3) = SUB(K,3)                             OUTP 178
      CALL EFMT(NPT,FSB,V)                          OUTP 179
330 CCNTINUE                                         OUTP 180

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331 WRITE(6,335) TRA          OUTP 199
335 FORMAT(83H0ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLOUTP 200
           1E FRACTIONS WERE LESS THAN ,E12.5,28H FOR ALL ASSIGNED CONDITIONS/OUTP 201
2/)          OUTP 202
LINE= 0          OUTP 203
NN = 1          OUTP 204
IF (EQL) NN=NPT          OUTP 205
DO 350 K=1,NS          OUTP 206
DO 340 I=1,NN          OUTP 207
IF ((EN(K,I)/TOTN(I)).GE.TRA) GO TO 343          OUTP 208
340 CONTINUE          OUTP 209
LINE= LINE+1          OUTP 210
Z (LINE, 1)= SUB(K, 1)          OUTP 211
Z (LINE, 2)= SUB(K, 2)          OUTP 212
Z (LINE, 3)= SUB(K, 3)          OUTP 213
343 IF ((LINE.NE.10) .AND. K.NE.NS) GO TO 350          OUTP 214
IF (LINE.EQ.0) GO TO 1000          OUTP 215
WRITE(6,345) (Z (LN,1),Z (LN,2),Z (LN,3),LN=1,LINE)          OUTP 216
345 FORMAT (10(1X,3A4))          OUTP 217
LINE= 0          OUTP 218
350 CONTINUE          OUTP 219
IF (.NCL.MOLES) WRITE(6,360)          OUTP 220
360 FORMAT(78H0NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIOOUTP 221
           2DANT IN TOTAL OXIDANTS )          OUTP 222
1000 RETURN          OUTP 223
END
SUBROUTINE THERMP          THRP 1
C
C      DOUBLE PRECISION HSUM,SSUM,CPR,DLVTP,DLVPT,GAMMAS          THRP 2
C      DOUBLE PRECISION COEF,S,EN,ENLN,H0,DELN          THRP 6
C
C      LOGICAL HP,SP,TP,UV,SV,NEWR,IONS,MOLES,FROZ,EQL,PSIA,RKT,VOL,TV          THRP 7
C      &,CALCH          THRP 8
C
C      DIMENSION VL(26)          THRP 9
C
C      COMMON/POINTS/HSUM(13),SSUM(13),CPR(13),DLVTP(13),DLVPT(13)          THRP 10
1 ,GAMMAS(13),P(26),T(26),V(13),PPP(13),WM(13),SONVEL(13),TTT(13)          THRP 11
2 ,VLM(13),TOTN(13)          THRP 12
COMMON/SPECES/COEF(2,7,250),S(250),EN(250,13),ENLN(250),H0(250)          THRP 13
1 ,DELN(250),A(15,250),SUB(250,3),IUSE(250),TEMP(50,2),SLN(250)          MAIN 22
COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),BOP(15,2)          THRP 23
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)          THRP 19
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)          THRP 20
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)          THRP 21
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENNL,ENSAVE,ENLSAV,TRACE,SIZE          REAC 11
COMMON/INDX/ IDEBUG,CONVG,TP,HP,SP,ISV, NPP, MOLES,NP,NT,NPT,NLM          THRP 24
1 ,NS,KMAT,IMAT,IQ1,NOF,NOMIT,IP,NEWR,NSUB,NSUP,ITM,CPCVFR,CPCVEQ          THRP 25
2 ,ICNS,NC,NSERT,JSOL,JLIQ,KASE,NREAC,IC,JS1,VOL,SHOCK,IT,NFZ,CALCH          THRP 26
3 ,IQSAVE,LSAVE,ISUP,ISUB,ITNUM          THRP 27
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)          THRP 28
1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2          THRP 29
2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO          THRP 30
C
C      EQUIVALENCE (K,ISV),(VL,P),(UV,HP),(TP,TV),(SP,SV)          THRP 31
C
C      DATA FUU/4HU, C/          THRP 32
C
C      IF(T(1).EQ.0.) T(1) = 3800.          THRP 33
C                                         THRP 34
C                                         THRP 35
C                                         THRP 36

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C
      IOF = 0
95  IOF = IOF+1
      OF = OXF(IOF)
      CALL NEWOF
      IF (TT.EQ.0..AND.CALCH) RETURN
C
C      SET ASSIGNED P OR VOLUME
C
      DO 902 IP=1,NP
      PP = P(IP)
      VLM(NPT) = VL(IP)
C
C      SET ASSIGNED T
C
      DO 902 IT=1,NT
      TT = T(IT)
      CALL EQLBRM
      IF (TT.NE.0.) GO TO 800
      IF (NPT.EQ.0) GO TO 1000
800  K = 0
      IF (IP.EQ.NP.AND.IT.EQ.NT.OR.TT.EQ.0.) GO TO 860
      K = NPT
      IF (NPT.NE.13) GO TO 870
860  IF (.NCT.HP) WRITE(6,5)
      5 FORMAT(1H1,41X,48HTHERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED
      1)
      IF (HP) WRITE(6,6)
      6 FORMAT(1H1,36X,59HTHERMODYNAMIC EQUILIBRIUM COMBUSTION PROPERTIES
      1AT ASSIGNED )
      IF (.NOT.VOL) GO TO 861
      IF (UV) WRITE(6,10)
      10 FORMAT(1H0,62X,7H VOLUME /)
      IF (TV) WRITE(6,11)
      11 FORMAT(1H0,54X,22H TEMPERATURE AND VOLUME/)
      IF (SV) WRITE(6,12)
      12 FORMAT(1H0,56X,18H ENTROPY AND VOLUME/)
      GO TO 862
861  IF (HP) WRITE(6,20)
      20 FORMAT(1H0,62X,10H PRESSURES /)
      IF (TP) WRITE(6,21)
      21 FORMAT(1H0,53X,24H TEMPERATURE AND PRESSURE/)
      IF (SP) WRITE(6,22)
      22 FORMAT(1H0,55X,20H ENTROPY AND PRESSURE/)
862  CALL CUT1
      WRITE (6,863)
863  FORMAT (25H0THERMODYNAMIC PROPERTIES//)
      IF (.NOT.VOL) GO TO 864
      FMT(4) = FMT(6)
      IF (.NOT.UV) GO TO 864
      DO 63 I=1,NPT
      FMT(2*I+3) = F2
      V(I) = HSUB0*R
63   CONTINUE
      WRITE(6,FMT) FUU,FH(2),FB,FB,(V(I),I=1,NPT)
864  CALL OUT2
      CALL CUT3
865  IF(K.EQ.0 .AND. IOF.EQ.NOF) GO TO 1000
      IF (IDEBUG.GT.13) IDEBUG=IDEBUG-13

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WRITE(6,868)	THRP	96
868 FORMAT(1H1)	THRP	97
NPT = 0	THRP	98
870 NPT = NPT + 1	THRP	99
IF(.NOT.TP.AND.TT.NE.0.) T(1)=TT	THRP	100
IF(NT.EQ.1.AND.NP.EQ.1) GO TO 95	THRP	101
IF(IP.EQ.1.AND.IT.EQ.1) ISV=-ISV	THRP	102
IF(NT.EQ.1) GO TO 871	THRP	103
IF(IT.EQ.NT.OR.TT.EQ.0.) ISV=0	THRP	104
871 CALL SAVE	THRP	105
902 CONTINUE	THRP	106
GO TO 95	THRP	108
1000 RETURN	THRP	109
END	THRP	110
BLOCK DATA	BLOK	1
C DIMENSION ATEM(3,50)	BLOK	2
C COMMON/MISC/ENN,SUMN,TT,SO,ATOM(3,101),LLMT(15),B0(15),B0P(15,2)	BLOK	5
1 ,TM,TLOW,TMID,THIGH,PP,CPSUM,OF,EQRAT,FPCT,R,RR,HSUB0,AC(2),AM(2)	BLOK	6
2 ,HPP(2),RH(2),VMIN(2),VPLS(2),WP(2),DATA(22),NAME(15,5)	BLOK	7
3 ,ANUM(15,5),PECWT(15),ENTH(15),FAZ(15),RTEMP(15),FOX(15),DENS(15)	BLOK	8
4 ,RHOP,RMW(15),TLN,CR,OXF(15),ENN,L,ENS,ENLSAV,TRACE,SIZE		
COMMON/OUPT/FMT(30),FP(4),FT(4),FH(4),FS(4),FM(4),FV(4),FD(4)	BLOK	10
1 ,FC(4),FG(4),FB,FMT13,F1,F2,F3,F4,F5,FL(4),FMTI9,FA1,FA2	BLOK	11
2 ,FR1,FC1,FN(4),FR(4),FA(4),FI(4),FMT9X,FO	BLOK	12
C EQUIVALENCE (ATOM(1,52),ATEM)	BLOK	13
C ATOMIC SYMBOLS, WEIGHTS, AND VALENCES	BLOK	15
C DATA ATOM/	BLOK	16
A 2HH , 1.00797 , 1., 2HHE , 4.0026 , 0., 2HLI , 6.939 , 1., BLOK	19	
B 2HBE , 9.0122 , 2., 2HB , 10.811 , 3., 2HC , 12.01115 , 4., BLOK	20	
C 2HN , 14.0067 , 0., 2HO , 15.9994,-2., 2HF , 18.9984 ,-1., BLOK	21	
D 2HNE , 20.183 , 0., 2HNA , 22.9898 , 1., 2HMG , 24.312 , 2., BLOK	22	
E 2HAL , 26.9815 , 3., 2HSI , 28.086 , 4., 2HP , 30.9738 , 5., BLOK	23	
F 2HS , 32.064 , 4., 2HCL , 35.453 ,-1., 2HAR , 39.948 , 0., BLOK	24	
G 2HK , 39.102 , 1., 2HCA , 40.080 , 2., 2HSC , 44.956 , 3., BLOK	25	
H 2HTI , 47.900 , 4., 2HV , 50.942 , 5., 2HCR , 51.996 , 3., BLOK	26	
I 2HMN , 54.9380 , 2., 2HFE , 55.847 , 3., 2HCO , 58.9332 , 2., BLOK	27	
J 2HNI , 58.710 , 2., 2HCU , 63.540 , 2., 2HZN , 65.370 , 2., BLOK	28	
K 2HGA , 69.720 , 3., 2HGE , 72.590 , 4., 2HAS , 74.9216 , 3., BLOK	29	
L 2HSE , 78.960 , 4., 2HBR , 79.909 ,-1., 2HKR , 83.800 , 0., BLOK	30	
M 2HRB , 85.47 , 1., 2HSR , 87.620 , 2., 2HY , 88.905 , 3., BLOK	31	
N 2HZR , 91.220 , 4., 2HNB , 92.906 , 5., 2HMO , 95.94 , 6., BLOK	32	
O 2HTC , 99.000 , 7., 2HRU , 101.070 , 3., 2HRH , 102.905 , 3., BLOK	33	
P 2HPD,106.400 , 2., 2HAG , 107.870 , 1., 2HCD , 112.400 , 2., BLOK	34	
Q 2HIN,114.820 , 3., 2HSN , 118.690 , 4., 2HSB , 121.750 , 3. , BLOK	35	
C DATA ATEM/	BLOK	36
R 2HTE,127.600 , 4., 2HI , 126.9044,-1., 2HXE , 131.300 , 0., BLOK	37	
S 2HCS,132.905 , 1., 2HBA , 137.340 , 2., 2HLA , 138.910 , 3., BLOK	38	
T 2HCE,140.120 , 3., 2HPR , 140.907 , 3., 2HND , 144.240 , 3., BLOK	39	
U 2HPM,145.000 , 3., 2HSM , 150.350 , 3., 2HEU , 151.960 , 3., BLOK	40	
V 2HGD,157.250 , 3., 2HTB , 158.924 , 3., 2HDY , 162.500 , 3., BLOK	41	
W 2HHO,164.930 , 3., 2HER , 167.260 , 3., 2HTM , 168.934 , 3., BLOK	42	
X 2HYB,173.040 , 3., 2HLU , 174.997 , 3., 2HHF , 178.490 , 4., BLOK	43	
Y 2HTA,180.948 , 5., 2HW , 183.850 , 6., 2HRE , 186.200 , 7., BLOK	44	
Z 2HOS,190.200 , 4., 2HIR , 192.200 , 4., 2HPT , 195.090 , 4., BLOK	45	

A	2HAU,196.967	, 3.,	2HHG,200.590	, 2.,	2HTL,204.370	, 1.,	BLOK	46
B	2HPB,207.190	, 2.,	2HBI,208.980	, 3.,	2HPO,210.000	, 2.,	BLOK	47
C	2HAT,210.000	, 0.,	2HRN,222.000	, 0.,	2HFR,223.000	, 1.,	BLOK	48
D	2HRA,226.000	, 2.,	2HAC,227.000	, 3.,	2HTH,232.038	, 4.,	BLOK	49
E	2HPA,231.000	, 5.,	2HU,238.030	, 6.,	2HNP,237.000	, 5.,	BLOK	50
F	2HPU,242.000	, 4.,	2HAM,243.000	, 3.,	2HCM,247.000	, 3.,	BLOK	51
G	2HBK,249.000	, 3.,	2HCF,251.000	, 3.,	2HES,254.000	, 0.,	BLOK	52
H	2HFM,253.000	, 0.,	2HD,2.014102,	1./			BLOK	53
							BLOK	54

C C INFORMATION USED IN VARIABLE OUTPUT FORMAT

C C BLOK 55

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DATA FMT/3H(1H,4H,3A4,4H,A2,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9BLOK0056
1.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9BLOK0057
2.,2H0,,3HF9.,2H0,,3HF9.,2H0,,3HF9.,1H0,1H)/, FB,F0,F1,F2,F3,F4,F5/BLOK0058
31H,,2H0,,2H1,,2H2,,2H3,,2H4,,2H5/,FMT13/2H13/,FMT9X/3H9X/,FMTI9BLOK0059
4/3HI9,/
      DATA           FP/4HP, A,4HTM ,2H ,1H /
1,FT/4HT, D,4HEG K,4H ,2H /,PH/4HH, C,4HAL/G,2H ,1H /
2,FS/4HS, C,4HAL/(,4HG) (K,2H) /,FM/4HM, M,4HOL W,2HT ,1H /
3,FV/4H(DLV,4H/DLP,4H) T ,2H /,FD/4H(DLV,4H/DT,2H) P,1H /
4,FC/4HCP, ,4HCAL/,4H(G) (,2HK)/,FG/4HGAMM,4HA (S,2H) ,1H /
5,FL/4HS0N ,4HVEL,,4HM/SE,2HC /

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BLOK 0060

C C INFORMATION USED IN PERFORMANCE OUTPUT

C C BLOK 61

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DATA FR1/4HPC/P/, FC1/2HCF/, FN/4HMACH,4H NUM,4HBER ,1H /
1,FR/4HCSTA,4HR, F,4HT/SE,2HC /,FI/4HISP,,4H LB-,4HSEC/,2HLB/
2,FA/4HIVAC,4H,LB-,4HSEC/,2HLB /,FA1/4HAE/A/,FA2/1HT/
END

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BLOK 62

BLOK 63

BLOK 64

BLOK 65

BLOK 66

BLOK 67

BLOK 68

BLOK 69

BLOK 70

BLOK 71

BLOK 72

Appendix C
DATA BASE LISTING

300.000	1000.000	5000.000						
AL(S)	J12/65AL	1.0	0.0	0.0	0.S	300.000	933.000	
0.0	0.0		0.0		0.0		0.0	
0.0	0.0		0.22258596E+01		0.25561699E-02		0.25963942E-06	
-0.44923993E-08	0.38348586E-11	-0.77250049E+03	-0.10016767E+02					
AL(L)	J12/65AL	1.0	0.0	0.0	0.L	933.000	5000.000	
0.38185053E+01	0.0		0.0		0.0		0.0	
-0.96116837E+02	-0.17518951E+02	0.38185053E+01	0.0		0.0		0.0	
0.0	0.0		-0.96116837E+02	-0.17518951E+02				
AL	J12/65AL	1.00	0.00	0.00	0.G	300.000	5000.000	
0.25450649E+01	-0.75157513E-04	0.48674178E-07	-0.14045399E-10		0.15219285E-14			
0.38498957E+05	0.53100252E+01	0.27964983E+01	-0.12468495E-02		0.20733314E-05			
-0.15487769E-08	0.43185442E-12	0.38456102E+05	0.41365423E+01					
AL+	J 6/65AL	1.E	-1.00	0.00	0.G	300.000	5000.000	
0.25138512E+01	-0.29077491E-04	0.20604308E-07	-0.59989574E-11		0.62050860E-15			
0.10859637E+06	0.37023325E+01	0.25006762E+01	-0.44314947E-05		0.10158061E-07			
-0.97918340E-11	0.33894328E-14	0.10860106E+06	0.37744970E+01					
ALB02	J 6/66AL	1.B	1.0	2.00	0.G	300.000	5000.000	
0.71722994E+01	0.29780741E-02	-0.12431110E-05	0.23188779E-09	-0.16041208E-13				
-0.67683687E+05	-0.99949245E+01	0.23087234E+01	0.18890537E-01	-0.20633350E-04				
0.10251323E-07	-0.16941283E-11	-0.66482187E+05	0.14463834E+02					
ALBR	J 6/72AL	1.BR	1.	0.	0.G	300.000	5000.000	
0.43850336E+01	0.20670501E-03	-0.67676979E-07	0.99615828E-11	0.20097773E-15				
0.57515942E+03	0.37106400E+01	0.36452732E+01	0.34206866E-02	-0.53309559E-05				
0.38278571E-08	-0.10286364E-11	0.71364966E+03	0.72229624E+01					
ALBR3(S)	J 6/72AL	1.BR	3.	0.	0.S	300.000	370.600	
0.0	0.0		0.0		0.0		0.0	
0.0	0.0		0.87219915E+01		0.39095506E-02		0.10929492E-04	
0.92093444E-07	-0.15291660E-09	-0.64454922E+05	-0.30179916E+02					
ALBR3(L)	J 6/72AL	1.BR	3.	0.	0.L	370.600	5000.000	
0.15030961E+02	0.0		0.0		0.0		0.0	
-0.64764930E+05	-0.60804733E+02	0.15030961E+02	0.0		0.0			
0.0	0.0		-0.64764930E+05	-0.60804733E+02				
ALBR3	J 6/72AL	1.BR	3.	0.	0.G	300.000	5000.000	
0.96298876E+01	0.41878945E-03	-0.18336431E-06	0.35402445E-10	-0.25141801E-14				
-0.52404820E+05	-0.13242801E+02	0.68052454E+01	0.12134213E-01	-0.18676525E-04				
0.13031411E-07	-0.33961393E-11	-0.51843781E+05	0.31669331E+00					
ALCL	J 6/70AL	1.CL	1.0	0.0	0.G	300.000	5000.000	
0.43563251E+01	0.21481038E-03	-0.63418383E-07	0.77108285E-11	0.34543444E-15				
-0.75342656E+04	0.24319992E+01	0.33408613E+01	0.43425038E-02	-0.63963589E-05				
0.42909178E-08	-0.10621486E-11	-0.73299687E+04	0.73232431E+01					
ALCL+	J 6/70AL	1.CL	1.E	-1.0	0.G	300.000	5000.000	
0.43784590E+01	0.18169187E-03	-0.48504688E-07	0.71019128E-11	-0.19982015E-15				
0.10181200E+06	0.30944624E+01	0.33659973E+01	0.43496378E-02	-0.65940530E-05				
0.45906177E-08	-0.11936528E-11	0.10201519E+06	0.79636469E+01					
ALCLF	J 9/64AL	1.CL	1.F	1.00	0.G	300.000	5000.000	
0.64598866E+01	0.59830281E-03	-0.25682112E-06	0.48695728E-10	-0.34023630E-14				
-0.62463695E+05	-0.33724194E+01	0.35819426E+01	0.11405580E-01	-0.15489626E-04				
0.93919219E-08	-0.20431530E-11	-0.61839641E+05	0.10712370E+02					
ALCLF2	J 9/64AL	1.CL	1.F	2.00	0.G	300.000	5000.000	
0.89238844E+01	0.11946920E-02	-0.51514911E-06	0.98204861E-10	-0.68997474E-14				
-0.12250081E+06	-0.15879099E+02	0.42218323E+01	0.18167324E-01	-0.23359622E-04				
0.13307893E-07	-0.26426994E-11	-0.12144556E+06	0.73068485E+01					
ALCL2	J 6/72AL	1.CL	2.	0.	0.G	300.000	5000.000	
0.66899223E+01	0.39869756E-03	-0.21062868E-06	0.50502186E-10	-0.39898640E-14				
-0.36805340E+05	-0.37500887E+01	0.45286112E+01	0.95054880E-02	-0.14786052E-04				
0.10422720E-07	-0.27462659E-11	-0.36383551E+05	0.65887995E+01					
ALCL2+	J 6/72AL	1.CL	2.E	-1.	0.G	300.000	5000.000	
0.71951561E+01	0.34419680E-03	-0.15048789E-06	0.29024602E-10	-0.20595909E-14				

0.45166746E+05-0.84473658E+01 0.51067762E+01 0.88177249E-02-0.13229385E-04
 0.90053831E-08-0.22846681E-11 0.45590430E+05 0.16231060E+01
 ALCL2- J 6/72AL 1.CL 2.E 1. 0.G 300.000 5000.000
 0.66721764E+01 0.38494356E-03-0.17212358E-06 0.31799258E-10-0.17301974E-14
 -0.48030535E+05-0.43962860E+01 0.43094416E+01 0.10247469E-01-0.15811631E-04
 0.11060994E-07-0.28912081E-11-0.47565297E+05 0.69281054E+01
 ALCL2F J 9/64AL 1.CL 2.F 1.00 0.G 300.000 5000.000
 0.91851568E+01 0.90569397E-03-0.39032125E-06 0.74305714E-10-0.52114210E-14
 -0.97869812E+05-0.15626927E+02 0.48609209E+01 0.17353740E-01-0.24017674E-04
 0.14983446E-07-0.34108046E-11-0.96939937E+05 0.54911547E+01
 ALCL3 (S) J 6/70AL 1.CL 3.0 0.0 0.S 300.000 465.700
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.98728294E+01 0.27331673E-02-0.26131733E-04
 0.144485909E-06-0.15684509E-09-0.87914062E+05-0.43727951E+02
 ALCL3 (L) J 6/70AL 1.CL 3.0 0.0 0.L 465.700 3000.000
 0.15096884E+02 0.0 0.0 0.0 0.0 0.0
 -0.85661750E+05-0.65219452E+02 0.15096884E+02 0.0 0.0 0.0
 0.0 0.0 -0.85661750E+05-0.65219452E+02
 ALCL3 J 6/70AL 1.CL 3.0 0.0 0.G 300.000 5000.000
 0.94303942E+01 0.634666863E-03-0.27374534E-06 0.52122182E-10-0.36552961E-14
 -0.73286437E+05-0.16464478E+02 0.56230669E+01 0.15859887E-01-0.23385655E-04
 0.15600602E-07-0.38581100E-11-0.72504000E+05 0.19471340E+01
 ALF J 6/69AL 1.F 1.0 0.0 0.G 300.000 5000.000
 0.41455460E+01 0.43007242E-03-0.16165006E-06 0.30017405E-10-0.20533756E-14
 -0.33233621E+05 0.19453516E+01 0.28306427E+01 0.47519319E-02-0.52178239E-05
 0.23098181E-08-0.23263553E-12-0.32918090E+05 0.85323219E+01
 ALF+ J 6/68AL 1.F 1.E -1.0 0.G 300.000 5000.000
 0.41987104E+01 0.38290909E-03-0.13075646E-06 0.22591318E-10-0.13164857E-14
 0.79682750E+05 0.24475603E+01 0.28575830E+01 0.50617419E-02-0.61248584E-05
 0.32221581E-08-0.54448503E-12 0.79991187E+05 0.90992308E+01
 ALF2 J 6/72AL 1.F 2. 0. 0.G 300.000 5000.000
 0.62152729E+01 0.89671346E-03-0.39959758E-06 0.78212131E-10-0.54296370E-14
 -0.90113000E+05-0.43882122E+01 0.30131922E+01 0.12349360E-01-0.15606303E-04
 0.86941476E-08-0.16652252E-11-0.89390375E+05 0.11424652E+02
 ALF2+ J 6/72AL 1.F 2.E -1. 0.G 300.000 5000.000
 0.68661060E+01 0.71111717E-03-0.30960211E-06 0.59534391E-10-0.42150596E-14
 0.34190066E+04-0.10385485E+02 0.37664127E+01 0.12302723E-01-0.16633378E-04
 0.10114203E-07-0.22270241E-11 0.40950486E+04 0.48008633E+01
 ALF2- J 6/72AL 1.F 2.E 1. 0.G 300.000 5000.000
 0.61635580E+01 0.93674078E-03-0.40458281E-06 0.75594170E-10-0.49244530E-14
 -0.11421394E+06-0.47997026E+01 0.29514494E+01 0.12074735E-01-0.14580574E-04
 0.75970732E-08-0.12762976E-11-0.11347162E+06 0.11149442E+02
 ALF3 (S) J 6/70AL 1.F 3.0 0.0 0.S 300.000 728.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.14269888E-01 0.44131409E-01-0.42722124E-04
 -0.27469991E-07 0.50384238E-10-0.18322250E+06-0.31981506E+01
 ALF3 (L) J 6/70AL 1.F 3.0 0.0 0.S 728.000 2500.000
 0.10355394E+02 0.24923489E-02-0.10104241E-05 0.33097525E-09-0.40272635E-13
 -0.18490487E+06-0.52032349E+02 0.92673512E+01 0.41513741E-02 0.17321754E-05
 -0.59286407E-08 0.29057616E-11-0.18458481E+06-0.46196716E+02
 ALF3 J 6/70AL 1.F 3.0 0.0 0.G 300.000 5000.000
 0.86469679E+01 0.15008084E-02-0.64734002E-06 0.12349330E-09-0.86836056E-14
 -0.14835750E+06-0.17033508E+02 0.36494102E+01 0.18770397E-01-0.22670923E-04
 0.11942436E-07-0.20760702E-11-0.14719481E+06 0.78078079E+01
 ALH J 6/63AL 1.H 1.00 0.00 0.G 300.000 5000.000
 0.33366899E+01 0.12877863E-02-0.49869942E-06 0.92294630E-10-0.63451679E-14
 0.30091762E+05 0.30823231E+01 0.36576853E+01-0.19744697E-02 0.68663394E-05
 -0.62041394E-08 0.18663101E-11 0.30146457E+05 0.20753460E+01
 ALI J 9/64AL 1.I 1. 0. 0.G 300.000 5000.000

0.44377747E+01 0.13030718E-03-0.30880745E-07 0.59579173E-11-0.42264191E-15
 0.58492422E+04 0.44447851E+01 0.38508053E+01 0.26700615E-02-0.42157990E-05
 0.30809695E-08-0.84329988E-12 0.59611328E+04 0.72378492E+01
 ALI3(S) J 6/64AL 1.I 3. 0. 0.S 300.000 464.150
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.50975098E+02 0.33522445E+00-0.40121420E-04
 -0.20644147E-05 0.26750062E-08-0.33786848E+05 0.22823021E+03
 ALI3(L) J 6/64AL 1.I 3. 0. 0.L 464.150 6000.000
 0.14593655E+02 0.0 0.0 0.0 0.0 0.0
 -0.39964473E+05-0.56754532E+02 0.14593655E+02 0.0 0.0 0.0
 0.0 0.0 -0.39964473E+05-0.56754532E+02
 ALI3 J 6/64AL 1.I 3. 0. 0.G 300.000 5000.000
 0.96933355E+01 0.34763361E-03-0.15241358E-06 0.29457575E-10-0.20937680E-14
 -0.27647766E+05-0.11867593E+02 0.71481104E+01 0.11088215E-01-0.17406812E-04
 0.12378859E-07-0.32924462E-11-0.27150641E+05 0.30693942E+00
 ALN(S) J12/62AL 1.N 1.00 0.00 0.S 300.000 3000.000
 0.47788458E+01 0.20198158E-02-0.12548671E-05 0.36283354E-09-0.39253241E-13
 -0.40062785E+05-0.26091965E+02-0.77586830E-01 0.17149061E-01-0.17948725E-04
 0.72995512E-08-0.55492557E-12-0.38837398E+05-0.15105476E+01
 ALN J 3/67AL 1.N 1.00 0.00 0.G 300.000 5000.000
 0.40281038E+01 0.56430930E-03-0.22198395E-06 0.42074941E-10-0.29421886E-14
 0.51028645E+05 0.21456699E+01 0.28422308E+01 0.39430186E-02-0.32512999E-05
 0.58151994E-09 0.29409157E-12 0.51340664E+05 0.82192669E+01
 ALO J 6/70AL 1.0 1.0 0.0 0.G 300.000 5000.000
 0.33971338E+01 0.88961166E-03 0.35688402E-06-0.19452653E-09 0.20793514E-13
 0.90775195E+04 0.67401133E+01 0.28793468E+01 0.34621619E-02-0.20990128E-05
 -0.67940387E-09 0.90680501E-12 0.90716797E+04 0.89123859E+01
 ALO+ J 6/70AL 1.0 1.E -1.0 0.G 300.000 5000.000
 0.89679966E+01-0.29837240E-02 0.66474632E-06-0.33205341E-10-0.27636991E-14
 0.11640681E+06-0.27398300E+02 0.52645836E+01-0.14004473E-01 0.38815982E-04
 -0.28971726E-07 0.55086864E-11 0.11903587E+06-0.16025820E+01
 ALOCL J 9/64AL 1.0 1.CL 1.00 0.G 300.000 5000.000
 0.67805204E+01 0.79662818E-03-0.34233358E-06 0.65022654E-10-0.45519212E-14
 -0.44080832E+05-0.93132973E+01 0.32444410E+01 0.14117006E-01-0.19322033E-04
 0.11962797E-07-0.27069180E-11-0.43312344E+05 0.79922152E+01
 ALOF J 3/64AL 1.0 1.F 1.00 0.G 300.000 5000.000
 0.64258966E+01 0.11928086E-02-0.51432841E-06 0.98028752E-10-0.68852835E-14
 -0.72744937E+05-0.93256979E+01 0.17646914E+01 0.17838839E-01-0.22537031E-04
 0.12468245E-07-0.23392217E-11-0.71691937E+05 0.13697771E+02
 ALCH J12/67AL 1.0 1.H 1.0 0.G 300.000 5000.000
 0.36860676E+01 0.33636822E-02-0.12466244E-05 0.21382204E-09-0.13898320E-13
 -0.23046105E+05 0.36769915E+01 0.26132212E+01 0.27716893E-02 0.74157833E-05
 -0.11354601E-07 0.45569555E-11-0.22586797E+05 0.10062166E+02
 ALCH+ J12/67AL 1.0 1.H 1.E -1.G 300.000 5000.000
 0.41501989E+01 0.28925212E-02-0.10565418E-05 0.17945168E-09-0.11587014E-13
 0.63892887E+05 0.26269922E+01 0.19603443E+01 0.79191141E-02-0.22857957E-05
 -0.40103778E-08 0.25707596E-11 0.64510184E+05 0.14093032E+02
 ALOH- J12/67AL 1.0 1.H 1.E 1.G 300.000 5000.000
 0.43010721E+01 0.21668503E-02-0.73988645E-06 0.11821055E-09-0.72208847E-14
 -0.29134094E+05 0.35138245E+01 0.29130201E+01 0.59530698E-02-0.30558058E-05
 -0.12598709E-08 0.12886090E-11-0.28781828E+05 0.10609284E+02
 ALO2 J 4/77AL 1.0 2.0 0.0 0.G 300.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.71949072E+01 0.12790336E-03-0.22525796E-07
 0.65654921E-11-0.50072564E-15-0.24987422E+05-0.12158555E+02
 ALO2- J 4/77AL 1.0 2.E 1.0 0.G 300.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.64186831E+01 0.80252206E-03-0.21504661E-06
 0.23750085E-10-0.86650263E-15-0.72762687E+05-0.93759947E+01

AL02H	J12/68AL	1.0	2.H	1.0	0.G	300.000	5000.000
0.64264345E+01	0.32230362E-02	-0.12139344E-05	0.21074500E-09	-0.13827999E-13			
-0.57626152E+05	-0.74707565E+01	0.24800453E+01	0.16149264E-01	-0.16033518E-04			
0.64466157E-08	-0.40994768E-12	-0.56682758E+05	0.12293907E+02				
AL2BR6	J 6/72AL	2.BR	6.	0.	0.G	300.000	5000.000
0.21264252E+02	0.83335303E-03	-0.36503491E-06	0.70489295E-10	-0.50060969E-14			
-0.11930300E+06	-0.56080963E+02	0.15101005E+02	0.26866771E-01	-0.42216634E-04			
0.30038223E-07	-0.79913185E-11	-0.11810062E+06	-0.26607101E+02				
AL2CL6	J 6/70AL	2.CL	6.0	0.0	0.G	300.000	5000.000
0.20777542E+02	0.13801872E-02	-0.60321543E-06	0.11629452E-09	-0.82492945E-14			
-0.16239444E+06	-0.62364319E+02	0.11794307E+02	0.38358845E-01	-0.58530262E-04			
0.40496491E-07	-0.10456811E-10	-0.16059681E+06	-0.19173370E+02				
AL2F6	J 6/70AL	2.F	6.0	0.0	0.G	300.000	5000.000
0.18970016E+02	0.33816486E-02	-0.14664311E-05	0.28107849E-09	-0.19847452E-13			
-0.32318862E+06	-0.64016846E+02	0.57619591E+01	0.51454931E-01	-0.66963315E-04			
0.38886878E-07	-0.79939883E-11	-0.32024150E+06	0.10213079E+01				
AL2O	J 6/72AL	2.O	1.	0.	0.G	300.000	5000.000
0.60079260E+01	0.11051758E-02	-0.47901534E-06	0.91824812E-10	-0.64862632E-14			
-0.18633816E+05	-0.43986044E+01	0.25541611E+01	0.12761232E-01	-0.14789648E-04			
0.72603612E-08	-0.10666806E-11	-0.17817965E+05	0.12833953E+02				
AL2C+	J 6/72AL	2.O	1.E	-1.	0.G	300.000	5000.000
0.60156574E+01	0.10963916E-02	-0.47515982E-06	0.91079186E-10	-0.64332491E-14			
0.71444062E+05	-0.40192060E+01	0.25845242E+01	0.12696780E-01	-0.14758130E-04			
0.72833544E-08	-0.10849949E-11	0.72253625E+05	0.13095532E+02				
AL2C2	J 9/65AL	2.O	2.00	0.00	0.G	300.000	5000.000
0.77227049E+01	0.25161623E-02	-0.10830290E-05	0.20637292E-09	-0.14502170E-13			
-0.51613930E+05	-0.13589237E+02	0.18895683E+01	0.19382190E-01	-0.16555045E-04			
0.32432492E-08	0.13877467E-11	-0.50096137E+05	0.16211777E+02				
AL2O2+	J 6/68AL	2.O	2.E	-1.0	0.G	300.000	5000.000
0.80829239E+01	0.21259699E-02	-0.91683421E-06	0.17488147E-09	-0.12295690E-13			
0.63056020E+05	-0.14431680E+02	0.18140841E+01	0.22238433E-01	-0.23492903E-04			
0.94504244E-08	-0.55539774E-12	0.64583715E+05	0.17091431E+02				
AL2O3 (S)	J 6/72AL	2.O	3.	0.	0.S	300.000	2327.000
0.12065894E+02	0.31581316E-02	0.40988681E-06	-0.80395623E-09	0.17762273E-12			
-0.20578231E+06	-0.64814163E+02	-0.23576698E+01	0.60831625E-01	-0.85195032E-04			
0.54358136E-07	-0.12629468E-10	-0.20288962E+06	0.47636690E+01				
AL2O3 (L)	J 6/72AL	2.O	3.	0.	0.L	2327.000	6000.000
0.20129181E+02	0.0	0.0	0.0	0.0	0.0		
-0.20365244E+06	-0.11488425E+03	0.0	0.0	0.0	0.0		
0.0	0.0	0.0	0.0	0.0	0.0		
AL2SI05 (S)	J 4/76AL	2.SI	1.0	5.	0.S	298.15	3000.00
0.0	0.0	0.0	0.0	0.0	0.0		
0.0	0.0	0.20029343E+02	0.30191217E-02	0.68621716E-06			
-0.27183034E-09	0.34311390E-13	-0.31871706E+06	-0.10619077E+03				
AL6SI2013 (S)	J 4/76AL	6.SI	2.0	13.	0.S	298.150	2023.00
0.0	0.0	0.0	0.0	0.0	0.0		
0.0	0.0	0.75958984E+02	-0.26140742E-01	0.17344675E-04			
-0.53496407E-08	0.98098873E-12	-0.84936687E+06	-0.40912085E+03				
AL6SI2013 (L)	J 4/76AL	6.SI	2.0	13.	0.L	2023.00	3000.00
0.0	0.0	0.0	0.0	0.0	0.0		
0.0	0.0	0.38584937E+03	-0.28257442E+00	0.51260518E-04			
0.13309549E-07	-0.35491826E-11	-0.11031110E+07	-0.23508049E+04				
AR	L 5/66AR	1.00	0.00	0.00	0.G	300.000	5000.000
0.25000000E+01	0.0	0.0	0.0	0.0	0.0		
-0.74537500E+03	0.43660002E+01	0.25000000E+01	0.0	0.0	0.0		
0.0	0.0	-0.74537500E+03	0.43660002E+01				
AR+	L12/66AR	1.E	-1.00	0.00	0.G	300.000	5000.000
0.28420668E+01	-0.87648601E-04	-0.26463209E-07	0.12240311E-10	-0.11885139E-14			
0.18272562E+06	0.36720200E+01	0.24856997E+01	-0.55682659E-03	0.33194847E-05			

-0.39236809E-08 0.14143279E-11 0.18290212E+06 0.58880157E+01
 AU(S) H11/76AU 1.0 0.0 0.0 0.S 298.150 1336.150
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.16051998E+01 0.39544292E-02-0.18673572E-05
 -0.15695547E-08 0.13127485E-11-0.56196143E+03-0.43360472E+01
 AU H11/76AU 1.0 0.0 0.0 0.G 298.150 3200.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.19828720E+01 0.77621522E-03-0.57716267E-06
 0.24637270E-09-0.32067512E-13 0.43835094E+05 0.10488758E+02
 B(S) J12/64B 1.0 0.0 0.0 0.S 300.000 2450.000
 0.21353846E+01 0.62384829E-03 0.52269843E-06-0.34412806E-09 0.54070294E-13
 -0.82167212E+03-0.12048934E+02-0.13181934E+01 0.11950485E-01-0.10999163E-04
 0.21567583E-08 0.12019864E-11-0.45597198E+02 0.51212196E+01
 B(L) J12/64B 1.0 0.0 0.0 0.L 2450.000 5000.000
 0.36735754E+01 0.0 0.0 0.0 0.0 0.0 0.0
 0.41164160E+03-0.21048340E+02 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 B J12/64B 1.00 0.00 0.00 0.G 300.000 5000.000
 0.25124741E+01-0.25820555E-04 0.18396001E-07-0.55496146E-11 0.61869870E-15
 0.66076125E+05 0.41307268E+01 0.25022984E+01-0.91340917E-06-0.15435319E-07
 0.26217528E-10-0.12048088E-13 0.66079750E+05 0.41856079E+01
 B+ J12/70B 1.E -1.0 0.0 0.G 300.000 5000.000
 0.25109701E+01-0.23555127E-04 0.17217943E-07-0.51879837E-11 0.55514815E-15
 0.16310594E+06 0.23465757E+01 0.24991665E+01 0.55246273E-05-0.12821246E-07
 0.12516710E-10-0.43867904E-14 0.16310975E+06 0.24093838E+01
 BCL J12/64B 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.41020575E+01 0.48659183E-03-0.18864324E-06 0.35833336E-10-0.25099069E-14
 0.15687957E+05 0.19420652E+01 0.28364468E+01 0.44368804E-02-0.43887521E-05
 0.15161079E-08 0.32646195E-13 0.16001359E+05 0.83321466E+01
 BCL+ J 6/68B 1.CL 1.E -1.0 0.G 300.000 5000.000
 0.41060886E+01 0.47274167E-03-0.17928585E-06 0.32416139E-10-0.20545758E-14
 0.14713100E+06 0.26295614E+01 0.28124199E+01 0.46006404E-02-0.48119964E-05
 0.19672215E-08-0.13837802E-12 0.14744850E+06 0.91435146E+01
 BCLF J12/64B 1.CL 1.F 1.00 0.G 300.000 5000.000
 0.57076759E+01 0.14100203E-02-0.60114138E-06 0.11367043E-09-0.79368071E-14
 -0.39693328E+05-0.15482178E+01 0.33120232E+01 0.74198768E-02-0.43485952E-05
 -0.11374057E-08 0.13763886E-11-0.39017547E+05 0.10935177E+02
 BCL2 J 6/72B 1.CL 2. 0. 0.G 300.000 5000.000
 0.64459839E+01 0.57927938E-03-0.26049707E-06 0.63596364E-10-0.53982223E-14
 -0.11661305E+05-0.44740400E+01 0.32974787E+01 0.12082577E-01-0.16123755E-04
 0.96265858E-08-0.20599199E-11-0.10956535E+05 0.11029363E+02
 BCL2+ J12/70B 1.CL 2.E -1.0 0.G 300.000 5000.000
 0.69266624E+01 0.67777629E-03-0.32101497E-06 0.68344427E-10-0.50073606E-14
 0.78857812E+05-0.89477873E+01 0.42704935E+01 0.10603789E-01-0.14229838E-04
 0.85372847E-08-0.18349671E-11 0.79436000E+05 0.40632906E+01
 BCL2- J 6/72B 1.CL 2.E 1. 0.G 300.000 5000.000
 0.63518219E+01 0.77028852E-03-0.44699863E-06 0.13831178E-09-0.13221995E-13
 -0.19705434E+05-0.47879009E+01 0.32358789E+01 0.11690218E-01-0.14778259E-04
 0.82181550E-08-0.15657909E-11-0.18981816E+05 0.10676830E+02
 BCL3 J12/64B 1.CL 3.00 0.00 0.G 300.000 5000.000
 0.85985384E+01 0.15531923E-02-0.67000605E-06 0.12789111E-09-0.90000063E-14
 -0.51357070E+05-0.15171594E+02 0.37395267E+01 0.18105812E-01-0.21340456E-04
 0.10828334E-07-0.17325967E-11-0.50214609E+05 0.90399628E+01
 BF J12/64B 1.F 1.00 0.00 0.G 300.000 5000.000
 0.35771885E+01 0.10192909E-02-0.41251565E-06 0.77196444E-10-0.53498736E-14
 -0.15127266E+05 0.32529087E+01 0.34613609E+01-0.95685478E-03 0.60135744E-05
 -0.64978067E-08 0.22355347E-11-0.14969820E+05 0.44475660E+01
 BF2 J 6/72B 1.F 2. 0. 0.G 300.000 5000.000
 0.54447460E+01 0.17533212E-02-0.78444475E-06 0.15719859E-09-0.11311071E-13

-0.72860375E+05-0.22865124E+01 0.30309305E+01 0.72411038E-02-0.28250915E-05
 -0.28920413E-08 0.20046100E-11-0.72151125E+05 0.10432510E+02
 BF2+ J12/70B 1.F 2.E -1.0 0.G 300.000 5000.000
 0.58127642E+01 0.18193424E-02-0.77103459E-06 0.14489782E-09-0.99809145E-14
 0.36794801E+05-0.70174885E+01 0.33146477E+01 0.86443648E-02-0.67525398E-05
 0.13383665E-08 0.45114910E-12 0.37483648E+05 0.58915129E+01
 BF2- J 6/72B 1.F 2.E 1. 0.G 300.000 5000.000
 0.53100348E+01 0.20020439E-02-0.97235534E-06 0.21641443E-09-0.16640880E-13
 -0.98336937E+05-0.23409710E+01 0.31424580E+01 0.64104572E-02-0.12386463E-05
 -0.41220112E-08 0.23472370E-11-0.97672937E+05 0.92120218E+01
 BF3 J 6/69B 1.F 3.0 0.0 0.G 300.000 5000.000
 0.70241985E+01 0.32221559E-02-0.13705157E-05 0.25919666E-09-0.18122311E-13
 -0.13918075E+06-0.11197486E+02 0.24468241E+01 0.15276313E-01-0.10784617E-04
 0.68907502E-09 0.14893191E-11-0.13790137E+06 0.12554636E+02
 BH J12/64B 1.H 1.00 0.00 0.G 300.000 5000.000
 0.28919077E+01 0.15832947E-02-0.58261730E-06 0.10242068E-09-0.67669564E-14
 0.52328715E+05 0.37829485E+01 0.36862202E+01-0.13055436E-02 0.26742109E-05
 -0.91073749E-09-0.15591136E-12 0.52176328E+05-0.68540394E-01
 BHF2 J12/65B 1.H 1.F 2.00 0.G 300.000 5000.000
 0.53184528E+01 0.47444478E-02-0.19337858E-05 0.35508374E-09-0.24293667E-13
 -0.90375000E+05-0.30563345E+01 0.24053602E+01 0.92755854E-02 0.13386461E-05
 -0.86807894E-08 0.41211019E-11-0.89388437E+05 0.12874850E+02
 BH2 J12/64B 1.H 2.00 0.00 0.G 300.000 5000.000
 0.33625288E+01 0.39012854E-02-0.15097548E-05 0.26672797E-09-0.17713051E-13
 0.22919027E+05 0.12459936E+01 0.23958282E+01 0.74776262E-02-0.72019511E-05
 0.45826383E-08-0.12510678E-11 0.23162648E+05 0.60631809E+01
 BH3 J12/64B 1.H 3.00 0.00 0.G 300.000 5000.000
 0.20621729E+01 0.72655901E-02-0.27510341E-05 0.47803717E-09-0.31334286E-13
 0.11923754E+05 0.88361664E+01 0.39487038E+01-0.52170549E-03 0.76481165E-05
 -0.46148685E-08 0.56318616E-12 0.11618809E+05-0.58801882E-01
 BN(S) J 6/66B 1.N 1.00 0.00 0.S 300.000 3500.000
 0.90909290E+00 0.81143267E-02-0.48032089E-05 0.12291916E-08-0.11517127E-12
 -0.30858566E+05-0.58284492E+01-0.11182451E+01 0.15038274E-01-0.11887860E-04
 0.21058502E-08 0.11962115E-11-0.30413090E+05 0.41742191E+01
 BN J 6/66B 1.N 1.00 0.00 0.G 300.000 5000.000
 0.35981836E+01 0.87176799E-03-0.29972642E-06 0.56036939E-10-0.40750416E-14
 0.56171242E+05 0.45869989E+01 0.35375061E+01-0.13556585E-02 0.62214185E-05
 -0.61683281E-08 0.19872463E-11 0.56329742E+05 0.55499506E+01
 BO J 6/68B 1.0 1.0 0.0 0.G 300.000 5000.000
 0.31564960E+01 0.13816589E-02-0.55049628E-06 0.99116673E-10-0.64164541E-14
 -0.10303423E+04 0.60242710E+01 0.37297249E+01-0.20878324E-02 0.57362849E-05
 -0.43894843E-08 0.10916632E-11-0.10618860E+04 0.36123219E+01
 BCCL J 3/65B 1.0 1.CL 1.00 0.G 300.000 5000.000
 0.57135563E+01 0.18664689E-02-0.77487897E-06 0.14398573E-09-0.99317730E-14
 -0.39977352E+05-0.48935833E+01 0.32705317E+01 0.10227751E-01-0.12070163E-04
 0.72025550E-08-0.16914742E-11-0.39378207E+05 0.73361225E+01
 BOF J 3/65B 1.0 1.F 1.00 0.G 300.000 5000.000
 0.52618484E+01 0.23462430E-02-0.97620796E-06 0.18167624E-09-0.12545889E-13
 -0.74324937E+05-0.40691032E+01 0.27741489E+01 0.93927644E-02-0.79998508E-05
 0.27457059E-08-0.11175219E-12-0.73640437E+05 0.87507486E+01
 BOF2 J12/66B 1.0 1.F 2.00 0.G 300.000 5000.000
 0.73077230E+01 0.29903620E-02-0.13059616E-05 0.25308244E-09-0.17687332E-13
 -0.10334575E+06-0.11205602E+02 0.17445974E+01 0.18693276E-01-0.15246164E-04
 0.26559470E-08 0.13798606E-11-0.10186756E+06 0.17339951E+02
 BO2 J 6/68B 1.0 2.0 0.0 0.G 300.000 5000.000
 0.58198433E+01 0.18626575E-02-0.81302795E-06 0.15735821E-09-0.10944238E-13
 -0.36255117E+05-0.65741062E+01 0.31212044E+01 0.84680878E-02-0.45972274E-05
 -0.16420021E-08 0.16658237E-11-0.35483309E+05 0.75346937E+01
 BC2- J12/68B 1.0 2.E 1.0 0.G 300.000 5000.000

0.48805170E+01 0.26743652E-02-0.10932190E-05 0.20080873E-09-0.13717770E-13
 -0.85284312E+05-0.30224934E+01 0.24916334E+01 0.97470656E-02-0.87640865E-05
 0.35802543E-08-0.40611221E-12-0.84641187E+05 0.92136784E+01
 BS J 6/72B 1.S 1. 0. 0.G 300.000 5000.000
 0.37068539E+01 0.98682893E-03-0.47495269E-06 0.10654601E-09-0.80519630E-14
 0.28012816E+05 0.44112129E+01 0.31742048E+01 0.98544965E-03 0.27711321E-05
 -0.43751811E-08 0.17616178E-11 0.28230625E+05 0.75204544E+01
 B2 J12/64B 2.00 0.00 0.00 0.G 300.000 5000.000
 0.39119968E+01 0.69145975E-03-0.27146626E-06 0.51110019E-10-0.35535912E-14
 0.96841812E+05 0.15798826E+01 0.29873314E+01 0.24872378E-02-0.94106611E-07
 -0.21308173E-08 0.11299017E-11 0.97128250E+05 0.65267344E+01
 B20 J 6/66B 2.0 1.00 0.00 0.G 300.000 5000.000
 0.47300539E+01 0.23941486E-02-0.10008325E-05 0.18697510E-09-0.12953671E-13
 0.98853359E+04-0.64909405E+00 0.35294733E+01 0.31993827E-02 0.30329256E-05
 -0.57491256E-08 0.22847349E-11 0.10363199E+05 0.62263889E+01
 B202 J12/64B 2.0 2.00 0.00 0.G 300.000 5000.000
 0.69938574E+01 0.35940392E-02-0.14753614E-05 0.27225133E-09-0.18695996E-13
 -0.57296180E+05-0.12180996E+02 0.36807079E+01 0.15361130E-01-0.18606093E-04
 0.12171451E-07-0.32411018E-11-0.56486648E+05 0.43429089E+01
 B203(L) J 6/71B 2.0 3.0 0.0 0.L 300.000 5000.000
 0.15600114E+02 0.0 0.0 0.0 0.0 0.0
 -0.15684456E+06-0.83126450E+02 0.31433273E+02-0.21578038E+00 0.64057996E-03
 -0.70572418E-06 0.26509150E-09-0.15490137E+06-0.12803880E+03
 B203 J 6/71B 2.0 3.0 0.0 0.G 300.000 5000.000
 0.83994102E+01 0.47436357E-02-0.19552308E-05 0.36187742E-09-0.24907231E-13
 -0.10357156E+06-0.15823207E+02 0.36608839E+01 0.20262077E-01-0.21947344E-04
 0.12253004E-07-0.27038406E-11-0.10236525E+06 0.80930147E+01
 B303CL3 J 3/65B 3.0 3.CL 3.00 0.G 300.000 5000.000
 0.19282562E+02 0.63172579E-02-0.27242922E-05 0.52047899E-09-0.36677790E-13
 -0.20320881E+06-0.67898331E+02 0.40444984E+01 0.54260597E-01-0.55750759E-04
 0.22223126E-07-0.14181295E-11-0.19941631E+06 0.90435429E+01
 B303F3 J 3/65B 3.0 3.F 3.00 0.G 300.000 5000.000
 0.16858612E+02 0.88685751E-02-0.37881055E-05 0.71870399E-09-0.50376919E-13
 -0.29093106E+06-0.59871948E+02 0.30798864E+01 0.45636591E-01-0.33098826E-04
 0.25538840E-08 0.44358761E-11-0.28712212E+06 0.11462196E+02
 BA(S) J12/70BA 1. 0. 0. 0.S 300.000 582.530
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.45722790E+01-0.17145739E-02-0.47855254E-04
 0.17441891E-06-0.13261330E-09-0.11469126E+04-0.17169785E+02
 BA(S) J12/70BA 1. 0. 0. 0.S 582.530 768.130
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.28171463E+01-0.52818879E-02 0.48730608E-05
 0.23825812E-07-0.19093449E-10-0.18129494E+03-0.62076797E+01
 BA(S) J12/70BA 1. 0. 0. 0.S 768.130 1000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.46986532E+01 0.0 0.0 0.0
 0.0 0.0 -0.13954702E+04-0.19397812E+02
 BA(L) J12/70BA 1. 0. 0. 0.L 1000.000 3500.000
 0.80692787E+01-0.39900132E-02 0.10720578E-05 0.64545105E-10-0.74451418E-14
 -0.21794053E+04-0.38283249E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 BA J12/70BA 1. 0. 0. 0.G 300.000 5000.000
 0.79730549E+01-0.11161216E-01 0.71172144E-05-0.15336672E-08 0.10876700E-12
 0.18889965E+05-0.23500809E+02 0.25038776E+01-0.37803911E-04 0.12914967E-06
 -0.18400409E-09 0.92934829E-13 0.20792543E+05 0.62036123E+01
 BACL J12/72BA 1.CL 1. 0. 0.G 300.000 5000.000
 0.46675234E+01-0.22187251E-03 0.81270684E-07 0.30216968E-10-0.53183301E-14
 -0.18542141E+05 0.44513073E+01 0.39781151E+01 0.21803218E-02-0.34342565E-05
 0.25182212E-08-0.69058030E-12-0.18366937E+05 0.79111271E+01

BACL2 (S) J12/72BA 1.CL 2. 0. 0.S 300.000 1198.000
 0.11096404E+02-0.11135002E-02-0.81801937E-06-0.23651370E-09 0.18326842E-11
 -0.10693775E+06-0.48926743E+02 0.77202473E+01 0.69224164E-02-0.10960927E-04
 0.96991606E-08-0.26198444E-11-0.10579200E+06-0.30768311E+02
 BACL2 (S) J12/72BA 1.CL 2. 0. 0.S 1198.000 1235.000
 0.14895592E+02 0.0 0.0 0.0 0.0
 -0.10994137E+06-0.75272705E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BACL2 (L) J12/72BA 1.CL 2. 0. 0.L 1235.000 5000.000
 0.13083967E+02 0.0 0.0 0.0 0.0
 -0.10578056E+06-0.60818649E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BACI2 J12/72BA 1.CL 2. 0. 0.G 300.000 5000.000
 0.69138641E+01 0.98213961E-04-0.43268347E-07 0.83969004E-11-0.59892090E-15
 -0.62076051E+05-0.31900012E+00 0.60571241E+01 0.38426148E-02-0.62683202E-05
 0.46196682E-08-0.12744771E-11-0.61914535E+05 0.37486544E+01
 BAF J12/72BA 1.F 1. 0. 0.G 300.000 5000.000
 0.43587122E+01 0.30110730E-03-0.22863316E-06 0.89865559E-10-0.87657610E-14
 -0.40101375E+05 0.45883512E+01 0.33537502E+01 0.43819584E-02-0.66405928E-05
 0.46143214E-08-0.11971518E-11-0.39892957E+05 0.94444551E+01
 BAF+ J12/72BA 1.F 1.E -1. 0.G 300.000 5000.000
 0.64945564E+01-0.41130073E-02 0.25882809E-05-0.50458704E-09 0.30719561E-13
 0.15960652E+05-0.78981133E+01 0.31617460E+01 0.48876069E-02-0.71219883E-05
 0.47144972E-08-0.11458985E-11 0.16960465E+05 0.95331039E+01
 BAF2 (S) J12/72BA 1.F 2. 0. 0.S 300.000 1480.000
 -0.28439283E+01-0.21997213E-01 0.44201064E-04 0.55824678E-08-0.13906912E-10
 -0.13789919E+06 0.44472931E+02 0.43203287E+01 0.27626146E-01-0.59430342E-04
 0.60630157E-07-0.22110799E-10-0.14745244E+06-0.19121918E+02
 BAF2 (S) J12/72BA 1.F 2. 0. 0.S 1480.000 1641.000
 0.12948094E+02 0.0 0.0 0.0 0.0
 -0.15033175E+06-0.65383667E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BAF2 (L) J12/72BA 1.F 2. 0. 0.L 1641.000 5000.000
 0.12006552E+02 0.0 0.0 0.0 0.0
 -0.14597712E+06-0.56701279E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BAF2 J12/72BA 1.F 2. 0. 0.G 300.000 5000.000
 0.67977161E+01 0.22932196E-03-0.10053520E-06 0.19428570E-10-0.13807507E-14
 -0.98763125E+05-0.27084208E+01 0.50968237E+01 0.74226260E-02-0.11682833E-04
 0.83296214E-08-0.22216855E-11-0.98431625E+05 0.54237833E+01
 BAO (S) J 6/74BA 1.0 1. 0. 0.S 300.000 2286.000
 0.55970564E+01 0.17242865E-02-0.60249511E-06 0.17400018E-09-0.18594792E-13
 -0.67719687E+05-0.23848526E+02 0.39200068E+01 0.89115649E-02-0.12531282E-04
 0.91868699E-08-0.26129073E-11-0.67394375E+05-0.15842468E+02
 BAO (L) J 6/74BA 1.0 1. 0. 0.L 2286.000 5000.000
 0.80516710E+01 0.0 0.0 0.0 0.0
 -0.63223738E+05-0.36818604E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BE (S) J 9/61BE 1.0 0.0 0.0 0.S 300.000 1556.000
 0.16386261E+01 0.18981069E-02-0.51915094E-08-0.40857562E-09 0.15576543E-12
 -0.54430884E+03-0.87156143E+01-0.53886199E+00 0.13250958E-01-0.19860265E-04
 0.13938457E-07-0.35115539E-11-0.27818237E+03 0.10351105E+01
 BE (L) J 9/61BE 1.0 0.0 0.0 0.L 1556.000 5000.000
 0.31549997E+01-0.46473346E-04 0.27783585E-06-0.89431670E-10 0.81533121E-14
 0.30546753E+03-0.16456528E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 BE J 9/61BE 1.00 0.00 0.00 0.G 300.000 5000.000
 0.24060354E+01 0.18872751E-03-0.11913204E-06 0.24933722E-10-0.56423639E-15
 0.38666156E+05 0.26445398E+01 0.24982462E+01 0.12910008E-04-0.33182303E-07

0.35564329E-10-0.13538107E-13 0.38633141E+05 0.21401110E+01
 BE+ J 6/65BE 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25101862E+01-0.21688742E-04 0.15756683E-07-0.47788232E-11 0.52465496E-15
 0.14754575E+06 0.27707491E+01 0.24942741E+01 0.41392108E-04-0.10472877E-06
 0.11080231E-09-0.41739398E-13 0.14754987E+06 0.28498688E+01
 BEBO2 J 6/66BE 1.B 1.0 2.00 0.G 300.000 5000.000
 0.69108372E+01 0.32668684E-02-0.13678118E-05 0.25576208E-09-0.17727742E-13
 -0.60505715E+05-0.91748505E+01 0.20069122E+01 0.18044826E-01-0.16917576E-04
 0.60865375E-08-0.17276285E-12-0.59234195E+05 0.15792365E+02
 BECL J 9/66BE 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.41052876E+01 0.47461712E-03-0.17996530E-06 0.32563910E-10-0.20652840E-14
 0.59753047E+04 0.24513645E+01 0.28321991E+01 0.44566765E-02-0.44482158E-05
 0.15852586E-08 0.45206894E-14 0.62906250E+04 0.88784075E+01
 BECL+ J 6/68BE 1.CL 1.E -1.0 0.G 300.000 5000.000
 0.53827496E+01-0.18471198E-02 0.11123684E-05-0.16952995E-09 0.61007108E-14
 0.11599719E+06-0.50753756E+01 0.28965988E+01 0.51267482E-02-0.64427913E-05
 0.35632639E-08-0.65925087E-12 0.11671469E+06 0.78241358E+01
 BECLF J 6/65BE 1.CL 1.F 1.00 0.G 300.000 5000.000
 0.64402790E+01 0.11463694E-02-0.48545360E-06 0.91287866E-10-0.63443547E-14
 -0.71059750E+05-0.77418556E+01 0.41024380E+01 0.85017495E-02-0.89093965E-05
 0.40076245E-08-0.51627539E-12-0.70468750E+05 0.40860071E+01
 BECL2(S) J 6/65BE 1.CL 2.00 0.00 0.S 300.000 688.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.30065746E+01 0.19539557E-01-0.48913607E-05
 -0.29604159E-07 0.23534855E-10-0.60722102E+05-0.12579772E+02
 BECL2(L) J 6/65BE 1.CL 2.00 0.00 0.L 688.000 5000.000
 0.14603719E+02 0.0 0.0 0.0 0.0
 -0.64498418E+05-0.76448792E+02 0.14603719E+02 0.0 0.0
 0.0 0.0 -0.64498418E+05-0.76448792E+02
 BECL2 J 6/65BE 1.CL 2.00 0.00 0.G 300.000 5000.000
 0.67043190E+01 0.87166461E-03-0.37255052E-06 0.70567011E-10-0.49335366E-14
 -0.45494559E+05-0.84351645E+01 0.44927130E+01 0.80535561E-02-0.88319239E-05
 0.40897064E-08-0.53498091E-12-0.44952883E+05 0.26826696E+01
 BEF J12/71BE 1.F 1. 0. G 300.000 5000.000
 0.37095299E+01 0.89383591E-03-0.36113067E-06 0.67601091E-10-0.46420828E-14
 -0.21660051E+05 0.31510296E+01 0.32761860E+01 0.25233766E-03 0.40939940E-05
 -0.53128133E-08 0.19954897E-11-0.21445926E+05 0.58518333E+01
 BEF2(S) J 6/70BE 1.F 2.0 0.0 0.S 300.000 500.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.20593765E+02-0.66396952E-01-0.12032398E-03
 0.89800557E-06-0.96669273E-09-0.12693706E+06-0.91785110E+02
 BEF2(S) J 6/70BE 1.F 2.0 0.0 0.S 500.000 825.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.56965580E+01 0.40258355E-02 0.0
 0.0 0.0 -0.12528881E+06-0.27091385E+02
 BEF2(L) J 6/70BE 1.F 2.0 0.0 0.L 825.000 2000.000
 0.60489635E+01 0.43328516E-02 0.18754400E-06-0.36019476E-09 0.91338829E-13
 -0.12511362E+06-0.29026245E+02 0.77423363E+01-0.69680065E-03 0.26743410E-05
 0.31262541E-08-0.25456278E-11-0.12546531E+06-0.37440308E+02
 BEF2 J 6/70BE 1.F 2.0 0.0 0.G 300.000 5000.000
 0.60457630E+01 0.15629374E-02-0.66108197E-06 0.12447551E-09-0.86716048E-14
 -0.97779125E+05-0.79310455E+01 0.35234270E+01 0.93890280E-02-0.95636206E-05
 0.42920973E-08-0.57751113E-12-0.97130437E+05 0.48708124E+01
 BEH J 3/63BE 1.H 1.00 0.00 0.G 300.000 5000.000
 0.30570221E+01 0.14977222E-02-0.56872960E-06 0.10260817E-09-0.69166983E-14
 0.37639512E+05 0.33871050E+01 0.37312307E+01-0.19143547E-02 0.48910324E-05
 -0.32925882E-08 0.66638562E-12 0.37565559E+05 0.37543893E+00
 BEH+ J 9/66BE 1.H 1.E -1.00 0.G 300.000 5000.000
 0.29015989E+01 0.16751762E-02-0.66805501E-06 0.12510951E-09-0.81741458E-14

0.13816812E+06 0.35425415E+01 0.37095709E+01-0.15852030E-02 0.36228766E-05
 -0.18933222E-08 0.17173264E-12 0.138C2869E+06-0.29598409E+00
 BEN J 6/63BE 1.N 1.00 0.00 0.G 300.000 5000.000
 0.37855940E+01 0.82386564E-03-0.32711603E-06 0.61551889E-10-0.42809045E-14
 0.50066180E+05 0.30924196E+01 0.31684284E+01 0.10282483E-02 0.27376018E-05
 -0.43481094E-08 0.17534455E-11 0.50310449E+05 0.66493587E+01
 BEO(S) J 6/71BE 1.0 1.0 0.0 0.S 300.000 2373.000
 0.40631027E+01 0.25962587E-02-0.81268058E-06 0.69616327E-10 0.14765804E-13
 -0.74752625E+05-0.22874329E+02-0.23035555E+01 0.26766192E-01-0.34874480E-04
 0.20738149E-07-0.43952429E-11-0.73402125E+05 0.81789389E+01
 BEO(S) J 6/71BE 1.0 1.0 0.0 0.S 2373.000 2720.000
 0.10599236E+02-0.33934040E-02-0.51791972E-07 0.67794659E-09-0.13472323E-12
 -0.78569812E+05-0.62792816E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 BEO(L) J 6/71BE 1.0 1.0 0.0 0.L 2720.000 5000.000
 0.75484419E+01 0.0 0.0 0.0 0.0 0.0
 -0.70795812E+05-0.42769379E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 BEO J 9/63BE 1.0 1.00 0.00 0.G 300.000 5000.000
 0.35048552E+01 0.10867885E-02-0.43990877E-06 0.82088961E-10-0.56778787E-14
 0.14435012E+05 0.33167343E+01 0.35250616E+01-0.13044281E-02 0.62838235E-05
 -0.63674968E-08 0.20911849E-11 0.14562191E+05 0.38321457E+01
 BEOH J 9/63BE 1.0 1.H 1.00 0.G 300.000 5000.000
 0.36351957E+01 0.28532436E-02-0.10230324E-05 0.17069994E-09-0.10840995E-13
 -0.13856066E+05 0.51296291E+01 0.37270355E+01-0.34554815E-03 0.82188517E-05
 -0.92269055E-08 0.32518302E-11-0.13732273E+05 0.53899403E+01
 BECH+ J 6/68BE 1.0 1.H 1.E -1.G 300.000 5000.000
 0.37549334E+01 0.33439584E-02-0.12505261E-05 0.21596827E-09-0.14114777E-13
 0.96194437E+05 0.14057045E+01 0.24619217E+01 0.36977984E-02 0.59446566E-05
 -0.10392931E-07 0.43387733E-11 0.96693750E+05 0.88341579E+01
 BEO2H2 J 3/67BE 1.0 2.H 2.00 0.G 300.000 5000.000
 0.64863234E+01 0.58388337E-02-0.21839205E-05 0.37665249E-09-0.24568933E-13
 -0.81124250E+05-0.93680115E+01 0.24681025E+01 0.18712513E-01-0.16655540E-04
 0.62752150E-08-0.30697537E-12-0.80137125E+05 0.10855417E+02
 BE2O J 9/63BE 2.0 1.00 0.00 0.G 300.000 5000.000
 0.54549732E+01 0.21970386E-02-0.92919578E-06 0.17496410E-09-0.12189983E-13
 -0.94958984E+04-0.56835861E+01 0.27527895E+01 0.89648701E-02-0.55859246E-05
 -0.34769188E-09 0.11015468E-11-0.87174727E+04 0.84387560E+01
 BE2OF2 J 6/66BE 2.0 1.F 2.00 0.G 300.000 5000.000
 0.10311343E+02 0.29258151E-02-0.12481987E-05 0.23652169E-09-0.16559159E-13
 -0.14844625E+06-0.24500839E+02 0.48600025E+01 0.19438982E-01-0.18818755E-04
 0.71009509E-08-0.37225258E-12-0.14703956E+06 0.32285700E+01
 BE2C2 J 9/63BE 2.0 2.00 0.00 0.G 300.000 5000.000
 0.71783648E+01 0.30796926E-02-0.13162271E-05 0.24970603E-09-0.17496340E-13
 -0.51984875E+05-0.12938758E+02 0.17102737E+01 0.18244941E-01-0.14377253E-04
 0.21268816E-08 0.14691989E-11-0.50512367E+05 0.15201347E+02
 BE3O3 J 9/63BE 3.0 3.00 0.00 0.G 300.000 5000.000
 C.91907320E+01 0.73623694E-02-0.31292730E-05 0.59162586E-09-0.41360195E-13
 -0.13061850E+06-0.23330048E+02 0.20002689E+01 0.20005170E-01 0.57517849E-06
 -0.17092805E-07 0.84862785E-11-0.12826869E+06 0.15607790E+02
 BE4O4 J 9/63BE 4.0 4.00 0.00 0.G 300.000 5000.000
 0.14547030E+02 0.81903748E-02-0.35162793E-05 0.66923467E-09-0.47005965E-13
 -0.19704844E+06-0.51509933E+02-0.13818436E+01 0.52384827E-01-0.40893021E-04
 0.47379700E-08 0.49954164E-11-0.19278356E+06 0.30399902E+02
 BI(S) BAR 73BI 1. 0. 0. 0.S 300.000 544.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.27582006E+01 0.12178153E-02 0.0
 0.0 0.0 -0.87648535E+03-0.92795773E+01
 BI(L) BAR 73BI 1. 0. 0. 0.L 544.000 5000.000

0.38245440E+01	0.0	0.0	0.0	0.0
0.32018143E+02	-0.12928786E+02	0.38245440E+01	0.0	0.0
0.0	0.0	0.32018143E+02	-0.12928786E+02	
BI	L 7/75BI	1.	0.	0.G 300.000 5000.000
0.24891729E+01	0.75025615E-04	-0.10964237E-06	0.50642796E-10	-0.51794676E-14
0.24162723E+05	0.82736969E+01	0.24992924E+01	0.49799301E-05	-0.12223765E-07
0.12502432E-10	-0.45306369E-14	0.24164559E+05	0.82376881E+01	
BIS	L 7/75BI	1.S	1.	0. 0.G 300.000 5000.000
0.43546543E+01	0.29133470E-03	-0.18135415E-06	0.59369204E-10	-0.55125209E-14
0.20302750E+05	0.67345057E+01	0.33705406E+01	0.50158612E-02	-0.90102249E-05
0.75182207E-08	-0.23759085E-11	0.20476922E+05	0.11328743E+02	
BI2S3 (S)	L 7/75BI	2.S	3.	0. S 300.000 1500.000
0.14543332E+02	0.30696997E-02	0.0	0.0	0.0
-0.38893430E+05	-0.59672577E+02	0.14543332E+02	0.30696997E-02	0.0
0.0	0.0	-0.38893430E+05	-0.59672577E+02	
BR	J 6/74BR	1.	0.	0.G 300.000 5000.000
0.20843210E+01	0.71949488E-03	-0.27419924E-06	0.42422649E-10	-0.23791569E-14
0.12858836E+05	0.90838003E+01	0.24611549E+01	0.33319276E-03	-0.10080657E-05
0.12262127E-08	-0.44283511E-12	0.12711922E+05	0.69494734E+01	
BR2(L)	J 9/61BR	2.0	0.0	0.0.L 265.900 1000.000
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.15501419E+02	-0.46806827E-01	0.11978985E-03
-0.12886306E-06	0.49440410E-10	-0.33667598E+04	-0.60333603E+02	
BR2	J12/61BR	2.0	0.0	0.0.G 300.000 5000.000
0.44479494E+01	0.10051209E-03	-0.16393816E-07	0.22685621E-11	-0.10236774E-15
0.23659941E+04	0.40888433E+01	0.38469582E+01	0.26111840E-02	-0.40034147E-05
0.28120688E-08	-0.73256201E-12	0.24846985E+04	0.69696989E+01	
C (S)	J 3/61C	1.0	0.0	0.0.S 300.000 5000.000
0.13604946E+01	0.19182237E-02	-0.84040391E-06	0.16448708E-09	-0.11672670E-13
-0.65713867E+03	-0.80070210E+01	-0.44778055E+00	0.53691007E-02	-0.39775568E-06
-0.40459298E-08	0.21134943E-11	-0.94280685E+02	0.16840792E+01	
C	J 3/61C	1.00	0.00	0.00.G 300.000 5000.000
0.25810661E+01	-0.14696202E-03	0.74388083E-07	-0.79481083E-11	0.58900977E-16
0.85216312E+05	0.43128881E+01	0.25328703E+01	-0.15887641E-03	0.30682082E-06
-0.26770075E-09	0.87488827E-13	0.85240437E+05	0.46062374E+01	
C+	L12/66C	1.E	-1.00	0.00.G 300.000 5000.000
0.25118275E+01	-0.17359780E-04	0.95042694E-08	-0.22188518E-11	0.18621892E-15
0.21667719E+06	0.42861300E+01	0.25953836E+01	-0.40686643E-03	0.68923669E-06
-0.52664872E-09	0.15083377E-12	0.21666281E+06	0.38957300E+01	
C-	J 9/65C	1.E	1.00	0.00.G 300.000 5000.000
0.24470587E+01	0.11286428E-03	-0.78591484E-07	0.19778609E-10	-0.11105555E-14
0.69973000E+05	0.42356997E+01	0.24925642E+01	0.53153068E-04	-0.13307994E-06
0.13951379E-09	-0.52150992E-13	0.69955750E+05	0.39811659E+01	
CCL	J12/69C	1.CL	1.0	0.0.G 300.000 5000.000
0.40984726E+01	0.50077843E-03	-0.20012834E-06	0.38680989E-10	-0.25441113E-14
0.59076598E+05	0.33370199E+01	0.31953554E+01	0.28076319E-02	-0.16043841E-05
-0.57744054E-09	0.61409731E-12	0.59325078E+05	0.80220194E+01	
CCL2	J12/68C	1.CI	2.0	0.0.G 300.000 5000.000
0.37185001E+01	0.53449757E-02	-0.23431285E-05	0.41806181E-09	-0.26765296E-13
0.27554793E+05	0.96328278E+01	0.28588505E+01	0.13957936E-01	-0.20038904E-04
0.13500728E-07	-0.31669719E-11	0.27363926E+05	0.12230161E+02	
CCL3	J 6/70C	1.CI	3.0	0.0.G 300.000 5000.000
0.87815475E+01	0.13516131E-02	-0.58249452E-06	0.11098697E-09	-0.77937263E-14
0.66344141E+04	-0.15329284E+02	0.37153358E+01	0.19443795E-01	-0.24627836E-04
0.13786465E-07	-0.26638934E-11	0.77820039E+04	0.97028913E+01	
CCL4	J12/68C	1.CL	4.0	0.0.G 300.000 5000.000
0.11601304E+02	0.15550272E-02	-0.67045278E-06	0.12770338E-09	-0.89616967E-14
-0.15389852E+05	-0.30063477E+02	0.42667398E+01	0.29452637E-01	-0.40820654E-04
0.25581546E-07	-0.58756489E-11	-0.13810816E+05	0.57614470E+01	

CF J 6/70C 1.F 1.0 0.0 0.G 300.000 5000.000
 0.36869678E+01 0.91143488E-03-0.36463854E-06 0.67482853E-10-0.45269608E-14
 0.29478125E+05 0.41613464E+01 0.34655142E+01-0.68779802E-03 0.56784766E-05
 -0.64582970E-08 0.22988252E-11 0.29655598E+05 0.58681917E+01
 CF+ J12/70C 1.F 1.E -1.0 0.G 300.000 5000.000
 0.36089983E+01 0.98626991E-03-0.39514129E-06 0.73142714E-10-0.49773181E-14
 0.13704675E+06 0.38918610E+01 0.34305944E+01-0.77491626E-03 0.58009482E-05
 -0.64435461E-08 0.22552099E-11 0.13721750E+06 0.53945580E+01
 CF2 J 6/70C 1.F 2.0 0.0 0.G 300.000 5000.000
 0.52267141E+01 0.20837679E-02-0.99037243E-06 0.21264848E-09-0.15831114E-13
 -0.23755848E+05-0.19240665E+01 0.27688818E+01 0.72372966E-02-0.16028152E-05
 -0.45512394E-08 0.26648007E-11-0.23015785E+05 0.11124533E+02
 CF2+ J12/70C 1.F 2.E -1.0 0.G 300.000 5000.000
 0.51554232E+01 0.20528310E-02-0.91173911E-06 0.18272761E-09-0.13213639E-13
 0.11143125E+06-0.79191321E+00 0.29783525E+01 0.60336590E-02 0.65858785E-09
 -0.52129465E-08 0.26663021E-11 0.11212675E+06 0.10938410E+02
 CF3 J 6/69C 1.F 3.0 0.0 0.G 300.000 5000.000
 0.72012625E+01 0.30663935E-02-0.13144181E-05 0.24996916E-09-0.17550929E-13
 -0.59238633E+05-0.10958873E+02 0.20650167E+01 0.16424157E-01-0.10838146E-04
 -0.85317997E-09 0.23878070E-11-0.57811977E+05 0.15691530E+02
 CF3+ J12/71C 1.F 3.E -1. 0.G 300.000 5000.000
 0.70225410E+01 0.32441271E-02-0.13864874E-05 0.26323632E-09-0.18464403E-13
 0.48022316E+05-0.11219685E+02 0.22605572E+01 0.15422322E-01-0.98956671E-05
 -0.78345042E-09 0.21211895E-11 0.49365340E+05 0.13565304E+02
 CF4 J 6/69C 1.F 4.0 0.0 0.G 300.000 5000.000
 0.91644297E+01 0.41978955E-02-0.17971488E-05 0.34132075E-09-0.23934115E-13
 -0.11571356E+06-0.23292953E+02 0.11656103E+01 0.27177785E-01-0.23317683E-04
 0.55706550E-08 0.12861856E-11-0.11360050E+06 0.17670654E+02
 CH J12/67C 1.H 1.0 0.0 0.G 300.000 5000.000
 0.22673120E+01 0.22042999E-02-0.62250189E-06 0.69689934E-10-0.21274952E-14
 0.70838062E+05 0.87889357E+01 0.35632753E+01-0.20031372E-03-0.40129817E-06
 0.18226922E-08-0.86768310E-12 0.70405500E+05 0.17628021E+01
 CH+ J12/71C 1.H 1.E -1. 0.G 300.000 5000.000
 0.27466402E+01 0.15496991E-02-0.52858326E-06 0.86132074E-10-0.50909763E-14
 0.19483675E+06 0.46994696E+01 0.35601597E+01-0.22478100E-03-0.26341621E-06
 0.16716215E-08-0.89478625E-12 0.19460362E+06 0.41570210E+00
 CH2 J12/72C 1.H 2. 0. 0.G 300.000 5000.000
 0.27525482E+01 0.39782040E-02-0.14921734E-05 0.25956903E-09-0.17110672E-13
 0.45547758E+05 0.66534796E+01 0.35883350E+01 0.21724137E-02-0.13323406E-05
 0.19469446E-08-0.89431392E-12 0.45315187E+05 0.22627869E+01
 CH20 J 3/61C 1.H 2.0 1.0 0.G 300.000 5000.000
 0.28364248E+01 0.68605281E-02-0.26882644E-05 0.47971249E-09-0.32118405E-13
 -0.15236031E+05 0.78531170E+01 0.37963781E+01-0.25701786E-02 0.18548817E-04
 -0.17869176E-07 0.55504455E-11-0.15088945E+05 0.47548161E+01
 CR3 J 6/69C 1.H 3.0 0.0 0.G 300.000 5000.000
 0.28400326E+01 0.60869083E-02-0.21740334E-05 0.36042569E-09-0.22725301E-13
 0.16449812E+05 0.55056753E+01 0.34666348E+01 0.38301845E-02 0.10116801E-05
 -0.18859236E-08 0.66803182E-12 0.16313105E+05 0.24172192E+01
 CH4 J 3/61C 1.H 4.00 0.00 0.G 300.000 5000.000
 0.15027075E+01 0.10416798E-01-0.39181523E-05 0.67777894E-09-0.44283706E-13
 -0.99787070E+04 0.10707143E+02 0.38261929E+01-0.39794594E-02 0.24558336E-04
 -0.22732927E-07 0.69626960E-11-0.10144949E+05 0.86690074E+00
 CN J 6/69C 1.N 1.0 0.0 0.G 300.000 5000.000
 0.36036282E+01 0.33644401E-03 0.10028936E-06-0.16318169E-10-0.36286722E-15
 0.51159832E+05 0.35454502E+01 0.37386303E+01-0.19239224E-02 0.47035192E-05
 -0.31113001E-08 0.61675318E-12 0.51270926E+05 0.34490213E+01
 CN+ J12/70C 1.N 1.E -1.0 0.G 300.000 5000.000
 0.36522923E+01 0.81427582E-03-0.20853349E-06 0.29071606E-10-0.17865094E-14
 0.21560181E+06 0.43916912E+01 0.36175022E+01-0.20179551E-02 0.79359852E-05

-0.77300619E-08 0.24798479E-11 0.21578131E+06 0.53579531E+01
 CN- J12/70C 1.N 1.E 1.0 0.G 300.000 5000.000
 0.29471722E+01 0.14988426E-02-0.57579547E-06 0.10177789E-09-0.67478507E-14
 0.63644336E+04 0.63743954E+01 0.37034311E+01-0.14896425E-02 0.31864702E-05
 -0.14831305E-08 0.48121663E-13 0.62335820E+04 0.27722845E+01
 CNN J 6/66C 1.N 2.00 0.00 0.G 300.000 5000.000
 0.48209076E+01 0.24790014E-02-0.94644111E-06 0.16548764E-09-0.10899129E-13
 0.68685937E+05-0.48484039E+00 0.35077782E+01 0.72023943E-02-0.75574590E-05
 0.42979202E-08-0.94257935E-12 0.68994250E+05 0.60234966E+01
 CN2 J12/70C 1.N 2.0 0.0 0.G 300.000 5000.000
 0.55626268E+01 0.20860606E-02-0.88123721E-06 0.16505783E-09-0.11366698E-13
 0.54897906E+05-0.55989351E+01 0.32524004E+01 0.70010722E-02-0.22653603E-05
 -0.28939808E-08 0.18270073E-11 0.55609086E+05 0.66966782E+01
 CO J 9/65C 1.0 1.00 0.00 0.G 300.000 5000.000
 0.29840698E+01 0.14891389E-02-0.57899683E-06 0.10364577E-09-0.69353533E-14
 -0.14245227E+05 0.63479156E+01 0.37100925E+01-0.16190964E-02 0.36923593E-05
 -0.20319675E-08 0.23953344E-12-0.14356309E+05 0.29555349E+01
 CCCC J12/65C 1.0 1.CL 1.00 0.G 300.000 5000.000
 0.54291239E+01 0.16121536E-02-0.66006282E-06 0.12127115E-09-0.82858592E-14
 -0.93305000E+04 0.36971813E+00 0.42863789E+01 0.50868988E-02-0.50729413E-05
 0.29647984E-08-0.77093453E-12-0.90125195E+04 0.62380304E+01
 COCL2 J 6/61C 1.0 1.CL 2.00 0.G 300.000 5000.000
 0.77318087E+01 0.24089287E-02-0.10111135E-05 0.18936214E-09-0.13139355E-13
 -0.29136566E+05-0.11221674E+02 0.31156139E+01 0.18478673E-01-0.22420543E-04
 0.12868185E-07-0.27360805E-11-0.28043883E+05 0.11755299E+02
 COF J12/65C 1.0 1.F 1.00 0.G 300.000 5000.000
 0.48908215E+01 0.22179703E-02-0.92550727E-06 0.17270120E-09-0.11955342E-13
 -0.22357984E+05 0.97962087E+00 0.32019730E+01 0.55837780E-02-0.14905481E-05
 -0.23126070E-08 0.13614353E-11-0.21817043E+05 0.10047576E+02
 COF2 J12/69C 1.0 1.F 2.0 0.G 300.000 5000.000
 0.65540361E+01 0.36729542E-02-0.15470214E-05 0.29065750E-09-0.20226547E-13
 -0.79321750E+05-0.81127748E+01 0.17973051E+01 0.16588710E-01-0.12553807E-04
 0.20091842E-08 0.11090061E-11-0.78009437E+05 0.16478043E+02
 COS J 3/61C 1.0 1.S 1.00 0.G 300.000 5000.000
 0.52391996E+01 0.24100584E-02-0.96064559E-06 0.17778347E-09-0.12235703E-13
 -0.18480453E+05-0.30910521E+01 0.24625320E+01 0.11947993E-01-0.13794370E-04
 0.80707743E-08-0.18327657E-11-0.17803988E+05 0.10792556E+02
 CO2 J 9/65C 1.0 2.00 0.00 0.G 300.000 5000.000
 0.44608040E+01 0.30981719E-02-0.12392575E-05 0.22741325E-09-0.15525955E-13
 -0.48961441E+05-0.98635983E+00 0.24007797E+01 0.87350942E-02-0.66070879E-05
 0.20021862E-08 0.63274039E-15-0.48377527E+05 0.96951456E+01
 CO2- J12/66C 1.0 2.E 1.00 0.G 300.000 5000.000
 0.45454636E+01 0.26054317E-02-0.10928734E-05 0.20454421E-09-0.14184542E-13
 -0.54761969E+05 0.18317366E+01 0.34743738E+01 0.16913805E-02 0.73533802E-05
 -0.99554249E-08 0.36846715E-11-0.54249051E+05 0.83834333E+01
 CP J 6/62C 1.P 1.00 0.00 0.G 300.000 5000.000
 0.37436113E+01 0.83811488E-03-0.34116215E-06 0.63775860E-10-0.44094638E-14
 0.54969176E+05 0.42305584E+01 0.32385855E+01 0.51754364E-03 0.35657386E-05
 -0.48985953E-08 0.18766551E-11 0.55196566E+05 0.72701283E+01
 CS J12/62C 1.S 1.00 0.00 0.G 300.000 5000.000
 0.36942530E+01 0.89086266E-03-0.36600045E-06 0.68778178E-10-0.47809995E-14
 0.26452215E+05 0.38176079E+01 0.33093033E+01 0.28164446E-04 0.44317876E-05
 -0.55253899E-08 0.20392464E-11 0.26658984E+05 0.62942705E+01
 CS2 J 6/61C 1.S 2.0 0.0 0.G 300.000 5000.000
 0.59867716E+01 0.16394437E-02-0.68384844E-06 0.12836890E-09-0.89167463E-14
 0.12043852E+05-0.63998222E+01 0.32144241E+01 0.10443848E-01-0.11062989E-04
 0.52967657E-08-0.83022695E-12 0.12745875E+05 0.76185760E+01
 C2 J12/69C 2.0 0.0 0.0 0.G 300.000 5000.000
 0.40435362E+01 0.20573653E-03 0.10907576E-06-0.36427875E-10 0.34127866E-14

0.99709500E+05 0.12775154E+01 0.74518137E+01-0.10144684E-01 0.85879738E-05
 0.87321106E-09-0.24429790E-11 0.98912000E+05-0.15846678E+02
 C2- J12/69C 2.E 1.0 0.0 0.G 300.000 5000.000
 0.36926260E+01 0.41576033E-03 0.11654212E-07 0.23755876E-11-0.14585314E-14
 0.52118953E+05 0.22470169E+01 0.37342911E+01-0.23034648E-02 0.68417830E-05
 -0.58120833E-08 0.16604296E-11 0.52281426E+05 0.27860422E+01
 C2CL2 J12/68C 2.CL 2.0 0.0 0.G 300.000 5000.000
 0.81728544E+01 0.23659891E-02-0.96552503E-06 0.17736149E-09-0.12135204E-13
 0.22510191E+05-0.14916744E+02 0.50229483E+01 0.14082666E-01-0.18095670E-04
 0.11610346E-07-0.28817478E-11 0.23227480E+05 0.59684169E+00
 C2F2 J12/67C 2.F 2.0 0.0 0.G 300.000 5000.000
 0.75164585E+01 0.31686462E-02-0.13311383E-05 0.24960056E-09-0.17342071E-13
 -0.16107655E+03-0.15081225E+02 0.35345840E+01 0.14445845E-01-0.12189692E-04
 0.36042984E-08 0.19118951E-12 0.92133569E+03 0.54063025E+01
 C2F4 J 6/69C 2.F 4.0 0.0 0.G 300.000 5000.000
 0.11086468E+02 0.52788444E-02-0.22354398E-05 0.42166848E-09-0.29433914E-13
 -0.83292875E+05-0.29880051E+02 0.36166182E+01 0.26488617E-01-0.22433262E-04
 0.62286460E-08 0.62149244E-12-0.81277250E+05 0.85106010E+01
 C2H J 3/67C 2.H 1.00 0.00 0.G 300.000 5000.000
 0.44207649E+01 0.22119302E-02-0.59294945E-06 0.94195776E-10-0.68527608E-14
 0.55835445E+05-0.11588097E+01 0.26499395E+01 0.84919520E-02-0.98165374E-05
 0.65373627E-08-0.17356273E-11 0.56275750E+05 0.76898613E+01
 C2HF J12/67C 2.H 1.F 1.0 0.G 300.000 5000.000
 0.60949497E+01 0.39432421E-02-0.14711441E-05 0.25294633E-09-0.16446663E-13
 0.12976906E+05-0.83285074E+01 0.26901770E+01 0.17680854E-01-0.22749853E-04
 0.14920570E-07-0.37381929E-11 0.13683223E+05 0.81338072E+01
 C2H2 J 3/61C 2.H 2.00 0.00 0.G 300.000 5000.000
 0.45751085E+01 0.51238351E-02-0.17452357E-05 0.28673064E-09-0.17951427E-13
 0.25607430E+05-0.35737944E+01 0.14102764E+01 0.19057274E-01-0.24501394E-04
 0.16390871E-07-0.41345443E-11 0.26188207E+05 0.11393827E+02
 C2H4 J 9/65C 2.H 4.00 0.00 0.G 300.000 5000.000
 0.34552155E+01 0.11491802E-01-0.43651753E-05 0.76155104E-09-0.50123198E-13
 0.44773125E+04 0.26987963E+01 0.14256821E+01 0.11383139E-01 0.79890006E-05
 -0.16253679E-07 0.67491256E-11 0.53370742E+04 0.14621819E+02
 C2H6 L 5/72C 2.H 6. 0. 0.G 300.000 1500.000
 0.21555281E+01 0.14779862E-01 0.23352804E-05-0.64146413E-08 0.19036925E-11
 -0.11524516E+05 0.10776316E+02 0.1415787E+01 0.10529719E-01 0.18730279E-04
 -0.26691186E-07 0.10049332E-10-0.11410484E+05 0.11647757E+02
 C2N J 3/67C 2.N 1.00 0.00 0.G 300.000 5000.000
 0.61931305E+01 0.14327539E-02-0.61255162E-06 0.11578707E-09-0.80401350E-14
 0.64818371E+05-0.84132299E+01 0.32670393E+01 0.98211318E-02-0.83284731E-05
 0.17650559E-08 0.59632767E-12 0.65589062E+05 0.65682306E+01
 C2N2 J 3/61C 2.N 2.00 0.00 0.G 300.000 5000.000
 0.65968933E+01 0.38694132E-02-0.15516162E-05 0.28141556E-09-0.19069442E-13
 0.34883727E+05-0.10001801E+02 0.39141779E+01 0.14011007E-01-0.17404353E-04
 0.12012780E-07-0.33565772E-11 0.35514551E+05 0.32384357E+01
 C2O J 9/66C 2.O 1.00 0.00 0.G 300.000 5000.000
 0.48990316E+01 0.28430384E-02-0.10209669E-05 0.16112164E-09-0.95542911E-14
 0.32800547E+05-0.91382283E+00 0.35364819E+01 0.69543868E-02-0.53071371E-05
 0.17030470E-08-0.14108072E-13 0.33151570E+05 0.60172367E+01
 C3 J12/69C 3.0 0.0 0.0 0.G 300.000 5000.000
 0.36815357E+01 0.24165236E-02-0.84348113E-06 0.14508197E-09-0.95697308E-14
 0.97413937E+05 0.68377800E+01 0.57408466E+01-0.84281228E-02 0.18620194E-04
 -0.14510530E-07 0.39676977E-11 0.97157500E+05-0.23837376E+01
 C302 J 6/68C 3.0 2.0 0.0 0.G 300.000 5000.000
 0.81435966E+01 0.54395013E-02-0.22192871E-05 0.40778625E-09-0.27915973E-13
 -0.14230012E+05-0.15456769E+02 0.37161007E+01 0.19872162E-01-0.20935753E-04
 0.11750114E-07-0.26589416E-11-0.13089402E+05 0.69298410E+01
 C4 J12/69C 4.0 0.0 0.0 0.G 300.000 5000.000

0. 65602102E+01 0. 40985234E-02 -0. 17000475E-05 0. 31615222E-09 -0. 21842144E-13
 0. 11430431E+06 -0. 11820311E+02 0. 18432016E+01 0. 19343592E-01 -0. 20627500E-04
 0. 10822625E-07 -0. 21289203E-11 0. 11550275E+06 0. 12006898E+02
 C5 J12/69C 5.0 0.0 0.0 0.G 300.000 5000.000
 0. 82067013E+01 0. 54889880E-02 -0. 22694876E-05 0. 42073367E-09 -0. 28981923E-13
 0. 11463650E+06 -0. 20246109E+02 0. 11012449E+01 0. 29513422E-01 -0. 33754346E-04
 0. 19056532E-07 -0. 40989018E-11 0. 11637969E+06 0. 15360193E+02
 CA(S) J12/68CA 1. 0. 0. 0.S 300.000 721.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.26381445E+01 0.25789358E-02 -0.27539227E-05
 -0.52522320E-09 0.15486518E-11 -0.87638696E+03 -0.10677312E+02
 CA(S) J12/68CA 1. 0. 0. 0.S 721.000 1112.000
 0. 32090769E+01 0. 30033942E-03 0. 10131916E-05 0. 44652637E-09 -0. 27724345E-12
 -0. 10618494E+04 -0. 13629311E+02 -0. 51791153E+01 0. 20122491E-01 -0. 11136081E-05
 -0. 22359298E-07 0. 13221420E-10 0. 11259233E+04 0. 29782791E+02
 CA(L) J12/68CA 1. 0. 0. 0.L 1112.000 5000.000
 0. 36232519E+01 0.0 0.0 0.0 0.0 0.0
 0. 23066978E+03 -0. 14552018E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 CA J12/68CA 1. 0. 0. 0.G 300.000 5000.000
 0. 17216101E+01 0. 17650847E-02 -0. 13531944E-05 0. 39990233E-09 -0. 33401379E-13
 0. 21071625E+05 0. 85348511E+01 0. 24999294E+01 0. 49376462E-06 -0. 12061696E-08
 0. 12304810E-11 -0. 44619028E-15 0. 20818016E+05 0. 43716621E+01
 CA+ J12/70CA 1.E -1. 0. 0.G 300.000 5000.000
 0. 23882484E+01 0. 34663593E-03 -0. 35813287E-06 0. 13674387E-09 -0. 13489925E-13
 0. 92530375E+05 0. 56266632E+01 0. 24998636E+01 0. 93965735E-06 -0. 22610143E-08
 0. 22602935E-11 -0. 79759015E-15 0. 92504062E+05 0. 50650654E+01
 CAAL2SI208(S) GS4/76CA 1.AL 2.SI 2.0 8.S 298.15 1700.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.31106354E+02 0.10505728E-01 -0.37120235E-05
 -0.14741632E-08 0.18698394E-11 -0.51916850E+06 -0.15944991E+03
 CABR2(S) J 6/74CA 1.BR 2. 0. 0.S 300.000 1015.000
 -0.86495002E+09 0.20238200E+07 -0.93777075E+03 -0.73663461E+00 0.51553571E-03
 0.24668183E+12 0.45365903E+10 0.15069797E+03 -0.10699205E+01 0.28421551E-02
 -0.32486969E-05 0.13343111E-08 -0.10726925E+06 -0.60225220E+03
 CABR2(L) J 6/74CA 1.BR 2. 0. 0.L 1015.000 5000.000
 0.13587196E+02 0.0 0.0 0.0 0.0 0.0
 -0.8542E750E+05 -0.63151657E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 CABR2 J 6/74CA 1.BR 2. 0. 0.G 300.000 5000.000
 0.74151640E+01 0.96549018E-04 -0.42463817E-07 0.82286868E-11 -0.58617052E-15
 -0.48536824E+05 -0.44939499E+01 0.66057158E+01 0.36058892E-02 -0.58314654E-05
 0.42634802E-08 -0.11667282E-11 -0.48382965E+05 -0.64420027E+00
 CACL J 6/70CA 1.CI 1. 0. 0.G 300.000 5000.000
 0.43067112E+01 0.40084962E-03 -0.23313663E-06 0.63921798E-10 -0.48662382E-14
 -0.13892656E+05 0.43602571E+01 0.36730518E+01 0.33144164E-02 -0.51682437E-05
 0.37111267E-08 -0.99687012E-12 -0.13784145E+05 0.73236790E+01
 CACL2(S) J 6/70CA 1.CI 2. 0. 0.S 300.000 1045.000
 0.87332411E+01 0.23955142E-03 0.94467379E-06 0.45851856E-09 -0.59749514E-13
 -0.98308062E+05 -0.37236664E+02 0.63554678E+01 0.13784312E-01 -0.24421402E-04
 0.19551280E-07 -0.49534170E-11 -0.98041812E+05 -0.26814148E+02
 CACL2(L) J 6/70CA 1.CI 2. 0. 0.L 1045.000 5000.000
 0.12332141E+02 0.0 0.0 0.0 0.0 0.0
 -0.98023937E+05 -0.58047470E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 CACL2 J 6/70CA 1.CI 2. 0. 0.G 300.000 5000.000
 0.73650017E+01 0.15327107E-03 -0.67275266E-07 0.13014131E-10 -0.92567974E-15
 -0.58954730E+05 -0.72016487E+01 0.61613359E+01 0.53060427E-02 -0.84649464E-05
 0.61128880E-08 -0.16522365E-11 -0.58722934E+05 -0.14614248E+01

CAF J12/68CA 1.F 1. 0. 0.G 300.000 5000.000
 0.41988621E+01 0.49244100E-03-0.26102123E-06 0.64791630E-10-0.47303944E-14
 -0.34021129E+05 0.34500351E+01 0.30508986E+01 0.51549450E-02-0.73508299E-05
 0.47876441E-08-0.11523152E-11-0.33792344E+05 0.89748964E+01
 CAF2(S) J12/68CA 1.F 2. 0. 0.S 300.000 1424.000
 0.72422428E+01 0.28310134E-02 0.14062443E-05-0.88232621E-09 0.24156366E-12
 -0.14964375E+06-0.33704407E+02 0.39744577E+01 0.25384068E-01-0.48742004E-04
 0.45090669E-07-0.14868440E-10-0.14940769E+06-0.20157120E+02
 CAF2(S) J12/68CA 1.F 2. 0. 0.S 1424.000 1691.000
 0.69984884E+01-0.62334836E-02 0.74337377E-05 0.52723301E-08-0.34396652E-11
 -0.14735000E+06-0.26874725E+02 0.0 0.0 0.0
 0.0 0.0 0.0
 CAF2(L) J12/68CA 1.F 2. 0. 0.L 1691.000 6000.000
 0.12017120E+02 0.0 0.0 0.0 0.0
 -0.14792856E+06-0.60511490E+02 0.0 0.0 0.0
 0.0 0.0 0.0
 CAF2 J12/68CA 1.F 2. 0. 0.G 300.000 5000.000
 0.66543427E+01 0.39052684E-03-0.17081072E-06 0.32952835E-10-0.23387740E-14
 -0.96445250E+05-0.53238459E+01 0.42308149E+01 0.10255806E-01-0.15444341E-04
 0.10546792E-07-0.26843918E-11-0.95955250E+05 0.63546820E+01
 CAI J 6/74CA 1.I 1. 0. 0.G 300.000 5000.000
 0.43198471E+01 0.43466687E-03-0.27441922E-06 0.80080442E-10-0.65451591E-14
 -0.19064805E+04 0.67016573E+01 0.40239105E+01 0.22559979E-02-0.40939831E-05
 0.34840051E-08-0.11162998E-11-0.18770510E+04 0.79771662E+01
 CAI2 J 6/74CA 1.I 2. 0. 0.G 300.000 5000.000
 0.74238663E+01 0.88555360E-04-0.39846892E-07 0.78918356E-11-0.57352664E-15
 -0.33287754E+05-0.29915981E+01 0.65641727E+01 0.42684637E-02-0.79247584E-05
 0.67205583E-08-0.21485461E-11-0.33138281E+05 0.10089397E+01
 CAO(S) J 6/73CA 1.0 1. 0. 0.S 300.000 3200.000
 0.56557512E+01 0.10165439E-02-0.25576901E-06 0.54514393E-10-0.42579940E-14
 -0.78238375E+05-0.28223373E+02 0.16937685E+01 0.18149663E-01-0.28372611E-04
 0.20513539E-07-0.55175768E-11-0.77482750E+05-0.93710079E+01
 CAO(L) J 6/73CA 1.0 1. 0. 0.L 3200.000 5000.000
 0.75484419E+01 0.0 0.0 0.0 0.0
 -0.71179312E+05-0.38083954E+02 0.0 0.0 0.0
 0.0 0.0 0.0
 CAO K11/74CA 1.0 1. 0. 0.G 300.000 5000.000
 0.36309423E+01 0.14765942E-02-0.63670825E-06 0.11672668E-09-0.78844131E-14
 0.81346055E+04 0.72235012E+01 0.28590889E+01 0.52468553E-02-0.73109486E-05
 0.51567639E-08-0.13720882E-11 0.82589102E+04 0.10783174E+02
 CAOH J 6/70CA 1.0 1.H 1. 0.G 300.000 5000.000
 0.53630466E+01 0.16592136E-02-0.59209088E-06 0.10693078E-09-0.70494690E-14
 -0.28499980E+05-0.25045834E+01 0.34961510E+01 0.10728817E-01-0.16114223E-04
 0.11340298E-07-0.29209916E-11-0.28219395E+05 0.60669651E+01
 CAOH+ J 6/70CA 1.0 1.H 1.E -1.G 300.000 5000.000
 0.54385204E+01 0.14831792E-02-0.45276272E-06 0.64638905E-10-0.35247383E-14
 0.42431344E+05-0.35995102E+01 0.34964495E+01 0.10726709E-01-0.16108999E-04
 0.11334865E-07-0.29189741E-11 0.42735926E+05 0.53725433E+01
 CAO2H2(S) J12/71CA 1.0 2.H 2. 0.S 300.000 3000.000
 0.10178703E+02 0.45142137E-02 0.44112642E-06-0.15806521E-09 0.20260323E-13
 -0.12191775E+06-0.49541611E+02 0.19381962E+01 0.48898865E-01-0.87004009E-04
 0.74579930E-07-0.23416727E-10-0.12071831E+06-0.12333704E+02
 CAS(S) J12/71CA 1.S 1. 0. 0.S 300.00 5000.00
 0.55426664E+01 0.99237799E-03 0.90343626E-08-0.22960557E-11 0.20031522E-15
 -0.58818027E+05-0.25082321E+02 0.42148819E+01 0.86643584E-02-0.16020014E-04
 0.14428220E-07-0.47454670E-11-0.58641715E+05-0.19191528E+02
 CASO4(S) J 4/76CA 1.S 1.0 4. 0.S 298.15 1400.00
 0.0 0.0 0.0 0.0 0.0
 0.0 -0.34144945E+01 0.47196943E-01-0.22226450E-04

-0.76269693E-08 0.67963404E-11-0.17353869E+06 0.19808594E+02
 CASIO3(S) GS4/76CA 1.SI 1.0 3. 0.S 298.15 1700.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.14101605E+02-0.18301302E-03 0.44535471E-06
 0.71887230E-09-0.28788045E-12-0.20069694E+06-0.71439789E+02
 CA2S1O4(S) GS4/76CA 2.SI 1.0 4. 0.S 298.15 970.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.83646727E+01 0.27587909E-01-0.56629706E-05
 -0.22813357E-07 0.14282514E-10-0.28112062E+06-0.40113770E+02
 CA2S1O4(S) GS4/76CA 2.SI 1.0 4. 0.S 970.00 1710.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.15829300E+02 0.45025386E-02 0.23290986E-05
 -0.16664532E-08 0.45634010E-12-0.28195137E+06-0.75899216E+02
 CA2S1O4(S) GS4/76CA 2.SI 1.0 4. 0.S 1710.00 2000.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.52679777E-02-0.81670709E-06 0.71406792E-09
 0.42517812E-12 0.271176941E+02-0.28494894E+06-0.14187300E+03
 CL J 6/72CL 1. 0. 0. 0.G 300.000 5000.000
 0.29537792E+01-0.40792720E-03 0.15288344E-06-0.26384339E-10 0.17206581E-14
 0.13695676E+05 0.30667324E+01 0.20774279E+01 0.29487170E-02-0.43919736E-05
 0.24499776E-08-0.41007687E-12 0.13871930E+05 0.73136339E+01
 CL+ J 6/65CL 1.E -1.00 0.00 0.G 300.000 5000.000
 0.31290607E+01-0.64678630E-03 0.25414317E-06-0.38607437E-10 0.20947135E-14
 0.16543856E+06 0.24486685E+01 0.19783297E+01 0.47071725E-02-0.86792897E-05
 0.63250312E-08-0.16313357E-11 0.16562587E+06 0.77975416E+01
 CL- J 6/65CL 1.E 1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0 0.0
 -0.28874559E+05 0.41872864E+01 0.25000000E+01 0.0 0.0 0.0
 0.0 0.0 -0.28874559E+05 0.41872873E+01
 CLCN J 6/66CL 1.C 1.N 1.00 0.G 300.000 5000.000
 0.54920025E+01 0.20987247E-02-0.77415916E-06 0.13823882E-09-0.92334858E-14
 0.14749160F+05-0.37436190E+01 0.33390856E+01 0.10397468E-01-0.13704650E-04
 0.95061949E-08-0.25925260E-11 0.15237539E+05 0.68178759E+01
 CLF J 9/65CL 1.F 1.00 0.00 0.G 300.000 5000.000
 0.41550341E+01 0.43195998E-03-0.16153996E-06 0.30453168E-10-0.21170113E-14
 -0.74382187E+04 0.22303896E+01 0.28480873E+01 0.47718994E-02-0.52877695E-05
 0.23634468E-08-0.24187423E-12-0.71277969E+04 0.87639112E+01
 CLF3 J 9/65CL 1.F 3.00 0.00 0.G 300.000 5000.000
 0.89535971E+01 0.11722164E-02-0.50896188E-06 0.97563485E-10-0.68858730E-14
 -0.22075969E+05-0.18094711E+02 0.28949118E+01 0.24718549E-01-0.35139325E-04
 0.22559590E-07-0.53261978E-11-0.20798641E+05 0.11368534E+02
 CLO J 6/61CL 1.0 1.00 0.00 0.G 300.000 5000.000
 0.40912619E+01 0.50003128E-03-0.18778206E-06 0.35097675E-10-0.24205038E-14
 0.10853223E+05 0.36057386E+01 0.28179359E+01 0.44531338E-02-0.44124890E-05
 0.15920942E-08-0.14486242E-13 0.11171398E+05 0.10044828E+02
 CLO2 J 3/61CL 1.0 2.00 0.00 0.G 300.000 5000.000
 0.57249756E+01 0.14645229E-02-0.59984353E-06 0.11388750E-09-0.79794773E-14
 0.10606266E+05-0.25921841E+01 0.28878164E+01 0.92875995E-02-0.70824044E-05
 0.63453376E-09 0.96801647E-12 0.11367379E+05 0.12006873E+02
 CL2 J 9/65CL 2.00 0.00 0.00 0.G 300.000 5000.000
 0.43077812E+01 0.31182822E-03-0.15310809E-06 0.44511908E-10-0.43057768E-14
 -0.13458252E+04 0.20666685E+01 0.31316891E+01 0.48997886E-02-0.69411462E-05
 0.44785651E-08-0.10621859E-11-0.10979695E+04 0.77833424E+01
 CL2O J12/65CL 2.0 1.00 0.00 0.G 300.000 5000.000
 0.64340057E+01 0.62728813E-03-0.26933253E-06 0.51076393E-10-0.35691529E-14
 0.84860547E+04-0.49498768E+01 0.32545242E+01 0.12799449E-01-0.17882456E-04
 0.11264383E-07-0.25964248E-11 0.91657422E+04 0.10558058E+02
 CO(S) J11/76CO 1. 0. 0. 0.S 298.000 1768.000
 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 -0.25391403E+02 0.48981313E-01-0.11657320E-04
 -0.12453619E-07 0.49695898E-11 0.95278437E+04 0.14311241E+03
 CC(L) J11/76CO 1. 0. 0. O.L 1768.000 4000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.10279985E+02-0.40723793E-02 0.75310146E-06
 0.58718350E-10-0.19291972E-13-0.51099062E+04-0.59104904E+02
 CO J11/76CO 1. 0. 0. O.G 298.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.30526505E+01 0.29656594E-03-0.19287944E-06
 0.43630197E-10-0.27112830E-14 0.50113184E+05 0.39657755E+01
 CR(S) J 6/73CR 1. 0. 0. O.S 300.000 2130.000
 0.28495474E+01-0.89168941E-04 0.11630091E-05-0.61538274E-10-0.34265535E-13
 -0.81093530E+03-0.13349285E+02 0.18820686E+01 0.38593342E-02-0.20938778E-05
 -0.15661770E-08 0.17462351E-11-0.71202026E+03-0.89298201E+01
 CR(L) J 6/73CR 1. 0. 0. O.L 2130.000 5000.000
 0.47279892E+01 0.28950799E-05-0.12765777E-08 0.24174158E-12-0.16665122E-16
 0.57713452E+03-0.24517990E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 CR J 6/73CR 1. 0. 0. O.G 300.000 5000.000
 0.35574541E+01-0.23813683E-02 0.16835465E-05-0.38473602E-09 0.31008711E-13
 0.46723973E+05 0.10637236E+01 0.25028009E+01-0.30550887E-04 0.11397145E-06
 -0.17493243E-09 0.94615505E-13 0.47061234E+05 0.66971416E+01
 CRN(S) J12/73CR 1.N 1. 0. O.S 300.000 2500.000
 0.56944542E+01 0.53011696E-03 0.22705831E-06-0.81483251E-10 0.10803797E-13
 -0.15836004E+05-0.28131699E+02 0.97152901E+01-0.23775373E-01 0.52561008E-04
 -0.48390746E-07 0.16270763E-10-0.16323422E+05-0.45730057E+02
 CRN J12/73CR 1.N 1. 0. O.G 300.000 5000.000
 0.38649607E+01 0.85160462E-03-0.44070759E-06 0.10667602E-09-0.83731409E-14
 0.59477437E+05 0.52819014E+01 0.29304638E+01 0.30377042E-02-0.12713963E-05
 -0.11781249E-08 0.85551347E-12 0.59744203E+05 0.10178715E+02
 CRO J12/73CR 1.O 1. 0. O.G 300.000 5000.000
 0.40139818E+01 0.62700245E-03-0.27956793E-06 0.60003100E-10-0.44057911E-14
 0.21346691E+05 0.55385494E+01 0.28414993E+01 0.40953346E-02-0.35776466E-05
 0.81710438E-09 0.24072010E-12 0.21646066E+05 0.11504827E+02
 CRO2 J12/73CR 1.O 2. 0. O.G 300.000 5000.000
 0.58499994E+01 0.12725100E-02-0.54920548E-06 0.10497490E-09-0.73995477E-14
 -0.11042184E+05-0.17581415E+01 0.33012648E+01 0.81625842E-02-0.58907681E-05
 0.16170856E-10 0.10816270E-11-0.10353570E+05 0.11385949E+02
 CRO3 J12/73CR 1.O 3. 0. O.G 300.000 5000.000
 0.81628942E+01 0.20450838E-02-0.88594129E-06 0.16976281E-09-0.11987766E-13
 -0.38092559E+05-0.15909059E+02 0.19072857E+01 0.23049608E-01-0.26501293E-04
 0.12862412E-07-0.18381989E-11-0.36608680E+05 0.15331977E+02
 CR2N(S) J12/73CR 2.N 1. 0. O.S 300.000 2500.000
 0.80984182E+01 0.18533610E-02 0.14227307E-05-0.55896399E-09 0.69307136E-13
 -0.17684801E+05-0.39147476E+02 0.20303392E+01 0.34006439E-01-0.61524945E-04
 0.53142546E-07-0.16769516E-10-0.16768312E+05-0.11600698E+02
 CR2O3(S) J12/73CR 2.O 3. 0. O.S 300.000 2603.000
 0.14012235E+02 0.13823977E-02-0.23779228E-06 0.16995085E-09-0.37705858E-13
 -0.14098219E+06-0.71101563E+02 0.29332779E+02-0.10207385E+00 0.23601102E-03
 -0.22578018E-06 0.77799295E-10-0.14240406E+06-0.13574281E+03
 CR2O3(L) J12/73CR 2.O 3. 0. O.L 2603.000 5000.000
 0.18871109E+02 0.0 0.0 0.0 0.0 0.0
 -0.13369500E+06-0.99961472E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 CS(S) J 6/68CS 1.0 0.0 0.0 O.S 300.000 301.550
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.31827765E+01-0.48708916E-02 0.18869585E-04
 0.89561411E-07-0.24031932E-09-0.96298877E+03-0.75956984E+01
 CS(L) J 6/68CS 1.0 0.0 0.0 O.I 301.550 1500.000

0.33149042E+01 0.82267355E-03-0.45641826E-06-0.95936037E-11 0.55471632E-13
 -0.70109814E+03-0.78759203E+01 0.47696838E+01-0.49137510E-02 0.84861113E-05
 -0.64184391E-08 0.18034315E-11-0.10158892E+04-0.14960727E+02
 CS J 6/68CS 1.0 0.0 0.0 0.G 300.000 5000.000
 0.18710098E+01 0.14068070E-02-0.10636222E-05 0.30583736E-09-0.19977218E-13
 0.86814570E+04 0.10235611E+02 0.24999466E+01 0.10382792E-05-0.38771191E-08
 0.49283910E-11-0.19810542E-14 0.84737812E+04 0.68627710E+01
 CS+ J12/70CS 1.E -1.0 0.0 0.G 300.000 5000.000
 0.25038681E+01-0.75238859E-05 0.47346482E-08-0.11801810E-11 0.10117554E-15
 0.54405152E+05 0.61482964E+01 0.25050507E+01-0.35642646E-04 0.88202967E-07
 -0.91546770E-10 0.33935528E-13 0.54406031E+05 0.61481752E+01
 CSCl(S) J 6/68CS 1.CL 1.0 0.0 0.S 300.000 743.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.55453396E+01 0.23805834E-02 0.83570330E-06
 -0.99571640E-09 0.38054802E-12-0.55026535E+05-0.20164261E+02
 CSCl(S) J 6/68CS 1.CL 1.0 0.0 0.S 743.000 918.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.81610737E+01-0.17623568E-02-0.22508516E-06
 0.39307351E-08-0.23452342E-11-0.55480430E+05-0.33941391E+02
 CSCl(L) J 6/68CS 1.CL 1.0 0.0 0.L 918.000 5000.000
 0.93097448E+01 0.0 0.0 0.0 0.0
 -0.55031160E+05-0.40810135E+02 0.93097448E+01 0.0 0.0
 0.0 0.0 -0.55031160E+05-0.40810135E+02
 CSCl J 6/68CS 1.CL 1.0 0.0 0.G 300.000 5000.000
 0.44798450E+01 0.10949164E-03-0.39989914E-08 0.20641995E-12 0.22184640E-16
 -0.30235809E+05 0.52041569E+01 0.41823034E+01 0.13759553E-02-0.20586931E-05
 0.14836474E-08-0.39764546E-12-0.30177926E+05 0.66253271E+01
 CSF(S) J 6/68CS 1.F 1.0 0.0 0.S 300.000 976.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.56489992E+01 0.18711397E-02 0.66242382E-06
 -0.63084871E-09 0.18692339E-12-0.68485125E+05-0.22149963E+02
 CSF(L) J 6/68CS 1.F 1.0 0.0 0.L 976.000 5000.000
 0.89071617E+01 0.0 0.0 0.0 0.0
 -0.68066812E+05-0.39912781E+02 0.89071617E+01 0.0 0.0
 0.0 0.0 -0.68066812E+05-0.39912781E+02
 CSF J 6/68CS 1.F 1.0 0.0 0.G 300.000 5000.000
 0.44373312E+01 0.12714999E-03-0.20547649E-07 0.29813357E-11-0.14774245E-15
 -0.44227996E+05 0.38603926E+01 0.37449875E+01 0.30100516E-02-0.45883817E-05
 0.32179694E-08-0.83786016E-12-0.44090695E+05 0.71817102E+01
 CSO J12/68CS 1.0 1.0 0.0 0.G 300.000 5000.000
 0.44660282E+01 0.11563233E-03-0.59989205E-08 0.13176699E-12 0.57639745E-16
 0.61950312E+04 0.52013855E+01 0.39857416E+01 0.21279252E-02-0.32170256E-05
 0.22764295E-08-0.59721976E-12 0.62898945E+04 0.75028591E+01
 CSOH(S) J 6/71CS 1.0 1.H 1.0 0.S 300.000 493.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.22667999E+02-0.79510629E-01-0.98326873E-05
 0.59683259E-06-0.72318240E-09-0.54096410E+05-0.96902542E+02
 CSOH(S) J 6/71CS 1.0 1.H 1.0 0.S 493.000 588.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.94903889E+01 0.20378267E-02-0.37207074E-05
 -0.24725999E-09 0.59676361E-11-0.52297613E+05-0.41264496E+02
 CSOH(I) J 6/71CS 1.0 1.H 1.0 0.L 588.000 5000.000
 0.98129749E+01 0.0 0.0 0.0 0.0
 -0.51757652E+05-0.41664444E+02 0.98129749E+01 0.0 0.0
 0.0 0.0 -0.51757652E+05-0.41664444E+02
 CSOH J 6/71CS 1.0 1.H 1.0 0.G 300.000 5000.000
 0.57005653E+01 0.11820383E-02-0.31939095E-06 0.38642922E-10-0.16635636E-14
 -0.32919203E+05-0.21318636E+01 0.45486002E+01 0.79612322E-02-0.13326497E-04
 0.10314235E-07-0.28973777E-11-0.32810891E+05 0.28487158E+01

CSCH+ J12/71CS 1.0 1.H 1.E -1.G 300.000 5000.000
 0.57292566E+01 0.11571324E-02-0.31044431E-06 0.37096284E-10-0.15509463E-14
 0.51626484E+05-0.58964044E+00 0.48487158E+01 0.68908334E-02-0.11839328E-04
 0.94335384E-08-0.27222686E-11 0.51678168E+05 0.30716906E+01
 CS2 J 6/68CS 2.0 0.0 0.0 0.G 300.000 5000.000
 0.46411467E+01 0.10844908E-03 0.10701307E-08 0.55978763E-10-0.77877429E-14
 0.11367605E+05 0.76209602E+01 0.45116577E+01 0.17392705E-03 0.36388656E-06
 -0.41459947E-09 0.16398514E-12 0.11426703E+05 0.83824692E+01
 CS2CL2 J 6/68CS 2.CL 2.0 0.0 0.G 300.000 5000.000
 0.99424372E+01 0.62659310E-04-0.26331097E-07 0.48912142E-11-0.33554151E-15
 -0.82345875E+05-0.10611221E+02 0.92952642E+01 0.28505600E-02-0.45576016E-05
 0.32557732E-08-0.86067362E-12-0.82222875E+05-0.75315142E+01
 CS2F2 J 6/68CS 2.F 2.0 0.0 0.G 300.000 5000.000
 0.98793726E+01 0.12674829E-03-0.50905253E-07 0.89711762E-11-0.58090959E-15
 -0.11005056E+06-0.14067985E+02 0.84425564E+01 0.64921007E-02-0.10832757E-04
 0.81791072E-08-0.23173980E-11-0.10978162E+06-0.72614079E+01
 CS20 J12/68CS 2.0 1.0 0.0 0.G 300.000 5000.000
 0.68979464E+01 0.10165098E-03-0.38062062E-07 0.61466396E-11-0.35758216E-15
 -0.13169988E+05-0.11790800E+01 0.57553635E+01 0.49116090E-02-0.77072518E-05
 0.54156963E-08-0.14080898E-11-0.12946828E+05 0.42869911E+01
 CS202H2 J 6/71CS 2.0 2.H 2.0 0.G 300.000 5000.000
 0.95809364E+01 0.53260513E-02-0.18780547E-05 0.30925928E-09-0.19429533E-13
 -0.86025812E+05-0.13227758E+02 0.75228195E+01 0.79078376E-02 0.35430303E-05
 -0.10456329E-07 0.48014032E-11-0.85338437E+05-0.19197969E+01
 CS2S04 RS6/77CS 2.S 1.0 4.0 0.G 298.15 3000.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.13779699E-03 0.28716881E-01-0.15754529E-04
 0.36285090E-08-0.28837311E-12-0.12100469E+06 0.90800903E+03
 CU(S) J11/76CU 1.0 0.0 0.0 0.S 298.000 1356.600
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.28439560E+01 0.50494564E-03 0.46544000E-06
 -0.56337135E-09 0.18073515E-12-0.88063745E+03-0.12408586E+02
 CU(L) J11/76CU 1.0 0.0 0.0 0.L 1356.60 4000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.64862432E+01-0.22913837E-02 0.56045525E-06
 -0.13614278E-10-0.64548451E-14-0.22874321E+04-0.34253052E+02
 CU J11/76CU 1.0 0.0 0.0 0.G 298.00 6000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.77080750E+00 0.18913769E-02-0.24387987E-06
 0.12021497E-10-0.23398819E-15 0.43566809E+05 0.27376465E+02
 E L02/67E 1.0 0.0 0.0 0.G 300.000 5000.000
 0.25C00000E+01 0.0 0.0 0.0 0.0
 -0.74537500E+03-0.11734026E+02 0.250000000E+01 0.0 0.0
 0.0 0.0 -0.74537500E+03-0.11734026E+02
 F J 9/65F 1.00 0.00 0.00 0.G 300.000 5000.000
 0.27004356E+01-0.22293182E-03 0.97941381E-07-0.19123036E-10 0.13768154E-14
 0.87163633E+04 0.38067179E+01 0.28128738E+01-0.33023098E-05-0.12897308E-05
 0.16837365E-08-0.64587832E-12 0.86604023E+04 0.30984201E+01
 F- J12/71F 1.E 1. 0. 0.G 300.000 5000.000
 0.25C00000E+01 0.0 0.0 0.0 0.0
 -0.31483637E+05 0.32516222E+01 0.250000000E+01 0.0 0.0
 0.0 0.0 -0.31483637E+05 0.32516222E+01
 FCN J 6/69F 1.C 1.N 1.0 0.G 300.000 5000.000
 0.50898561E+01 0.24170685E-02-0.97682732E-06 0.17813442E-09-0.12118568E-13
 0.25780781E+04-0.28859453E+01 0.32516937E+01 0.83073154E-02-0.83666355E-05
 0.44125628E-08-0.90882423E-12 0.30551199E+04 0.64289827E+01
 FO J12/66F 1.0 1.00 0.00 0.G 300.000 5000.000
 0.39192772E+01 0.70442352E-03-0.26648206E-06 0.49617602E-10-0.33688571E-14
 0.11798191E+05 0.33155947E+01 0.29680023E+01 0.26483394E-02-0.37368005E-06

-0.19006225E-08 0.10614287E-11 0.12087844E+05 0.83803339E+01
 F02 J 9/66F 1.0 2.00 0.00 0.G 300.000 5000.000
 0.57040939E+01 0.13862888E-02-0.58355374E-06 0.10937214E-09-0.75869182E-14
 -0.39678687E+03-0.20810804E+01 0.37805071E+01 0.68174601E-02-0.58133601E-05
 0.17562505E-08 0.67757432E-13 0.12769469E+03 0.78225203E+01
 F2 J12/60F 2.0 0.0 0.0 0.G 300.000 5000.000
 0.40397806E+01 0.60869032E-03-0.21494674E-06 0.40596804E-10-0.28294433E-14
 -0.13123535E+04 0.99528039E+00 0.28445997E+01 0.40135086E-02-0.32165653E-05
 0.47418780E-09 0.35556237E-12-0.99911768E+03 0.71131620E+01
 F20 J12/69F 2.0 1.0 0.0 0.G 300.000 5000.000
 0.60051870E+01 0.11028403E-02-0.47547940E-06 0.90683142E-10-0.63757085E-14
 0.91906055E+03-0.52352686E+01 0.26109219E+01 0.12231279E-01-0.13441415E-04
 0.58909428E-08-0.57487175E-12 0.17347195E+04 0.11774719E+02
 FE(S) J 3/65FE 1.00 0.00 0.00 0.S 300.000 1184.000
 0.40283340E+02-0.25054768E-01-0.24866007E-04 0.11749265E-07 0.47159221E-11
 -0.20310191E+05-0.23775826E+03 0.32514000E+01-0.72791651E-02 0.34254204E-04
 -0.49586131E-07 0.26187441E-10-0.83324316E+03-0.14209130E+02
 FE(S) J 3/65FE 1.00 0.00 0.00 0.S 1184.000 1665.000
 0.32005396E+01 0.75484416E-03 0.0 0.0 0.0 0.0
 -0.17210443E+03-0.14410926E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 FE(S) J 3/65FE 1.00 0.00 0.00 0.S 1665.000 1809.000
 0.34018316E+01 0.90581295E-03 0.0 0.0 0.0 0.0
 -0.58567529E+03-0.16076797E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 FE(L) J 3/65FE 1.00 0.00 0.00 0.O.L 1809.000 5000.000
 0.49215841E+01 0.20129178E-03 0.0 0.0 0.0 0.0
 -0.35541943E+03-0.25191483E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 FE J 3/65FE 1.00 0.00 0.00 0.G 300.000 5000.000
 0.34436541E+01-0.14011625E-02 0.81291353E-06-0.16290473E-09 0.12250807E-13
 0.49122684E+05 0.25061140E+01 0.26358461E+01 0.37581262E-02-0.99073795E-05
 0.9094270E-08-0.28812664E-11 0.49187398E+05 0.59230480E+01
 FECL J 6/65FE 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.46940670E+01 0.11604078E-03-0.20840176E-07-0.17626560E-11 0.52313814E-15
 0.28790344E+05 0.41803970E+01 0.37885828E+01 0.43678023E-02-0.66922330E-05
 0.41707438E-08-0.84686771E-12 0.28920098E+05 0.83402100E+01
 FECL2(S) J12/70FE 1.CL 2.0 0.0 0.S 300.000 950.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.71122274E+01 0.11086952E-01-0.17072744E-04
 0.13515816E-07-0.41365036E-11-0.43600984E+05-0.28994049E+02
 FECL2(L) J12/70FE 1.CL 2.0 0.0 0.L 950.000 5000.000
 0.12288863E+02 0.0 0.0 0.0 0.0 0.0
 -0.41109820E+05-0.53193054E+02 0.12288863E+02 0.0 0.0 0.0
 0.0 0.0 -0.41109820E+05-0.53193054E+02
 FECL2 J12/70FE 1.CL 2.0 0.0 0.G 300.000 5000.000
 0.69492598E+01 0.53371652E-03 0.70221233E-07-0.61475491E-10 0.67933127E-14
 -0.19045832E+05-0.37726707E+01 0.54557505E+01 0.79632923E-02-0.12593964E-04
 0.89976737E-08-0.23242363E-11-0.18844297E+05 0.30096865E+01
 FECL3(S) J 6/65FE 1.CL 3.00 0.00 0.S 300.000 577.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.11806993E+02 0.18280681E-01-0.19156683E-03
 0.57778465E-06-0.49460658E-09-0.51600496E+05-0.51237244E+02
 FECL3(L) J 6/65FE 1.CL 3.00 0.00 0.L 577.000 1500.000
 0.16102570E+02 0.0 0.0 0.0 0.0 0.0
 -0.48435531E+05-0.67614578E+02 0.16102570E+02 0.0 0.0 0.0
 0.0 0.0 -0.48435531E+05-0.67614578E+02
 FECL3 J 6/65FE 1.CL 3.00 0.00 0.G 300.000 5000.000
 0.97771111E+01 0.24421373E-03-0.10313994E-06 0.19207427E-10-0.13179299E-14

-0.33439570E+05-0.14562301E+02 0.75614872E+01 0.97338259E-02-0.15543308E-04
 0.11186369E-07-0.30022998E-11-0.33013625E+05-0.39989862E+01
FEO (S) J 6/65FE 1.0 1.00 0.00 0.S 300.000 1650.000
 0.58316488E+01 0.14275156E-02-0.93208143E-07-0.65997763E-11-0.22512144E-13
 -0.34566902E+05-0.26446991E+02 0.53195477E+01 0.22096592E-02 0.10721778E-05
 -0.27929730E-08 0.13320733E-11-0.34407164E+05-0.23686035E+02
FEO(L) J 6/65FE 1.0 1.00 0.00 0.L 1650.000 5000.000
 0.82022486E+01 0.0 0.0 0.0 0.0 0.0
 -0.33848613E+05-0.40079132E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
FEO J 9/66FE 1.0 1.00 0.00 0.G 300.000 5000.000
 0.42049818E+01 0.26838458E-03-0.89426749E-07 0.31855907E-10-0.33922543E-14
 0.28829172E+05 0.48172684E+01 0.28245258E+01 0.43049194E-02-0.41084777E-05
 0.13201189E-08 0.71316217E-13 0.29194035E+05 0.11878013E+02
FEO2H2(S) J 6/66FE 1.0 2.H 2.00 0.S 300.000 1500.000
 0.74031811E+01 0.11981741E-01-0.14957614E-05-0.50526374E-08 0.20037114E-11
 -0.71592250E+05-0.34673264E+02 0.10091218E+02 0.44523142E-02 0.40666855E-05
 -0.40094541E-08 0.23947164E-12-0.72277687E+05-0.48400040E+02
FEO2H2 J12/66FE 1.0 2.H 2.00 0.G 300.000 5000.000
 0.87960424E+01 0.45844391E-02-0.18808769E-05 0.34177394E-09-0.23047933E-13
 -0.42754562E+05-0.17856567E+02 0.14918175E+01 0.38499266E-01-0.61500978E-04
 0.46635112E-07-0.13306872E-10-0.41450949E+05 0.16384308E+02
FE03H3(S) J 6/66FE 1.0 3.H 3.00 0.S 300.000 1500.000
 0.80223923E+01 0.16420133E-01-0.12369378E-06-0.68192847E-08 0.23276910E-11
 -0.10321337E+06-0.37934021E+02 0.44116840E+01 0.32682464E-01-0.22393811E-04
 0.28646792E-08 0.22622321E-11-0.10271831E+06-0.21331009E+02
FES(S) BAR 73FE 1.S 1. 0. 0.S 300.000 411.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.13049394E+02-0.56390386E-01 0.11069136E-03
 0.0 0.0 -0.14389398E+05-0.55205719E+02
FES(S) BAR 73FE 1.S 1. 0. 0.S 411.000 598.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.87561932E+01 0.0 0.0 0.0
 0.0 0.0 -0.14539176E+05-0.42496185E+02
FES(S) BAR 73FE 1.S 1. 0. 0.S 598.000 1468.000
 0.61393995E+01 0.11976862E-02 0.0 0.0 0.0 0.0
 -0.13128094E+05-0.26380707E+02 0.61393995E+01 0.11976862E-02 0.0
 0.0 0.0 -0.13128094E+05-0.26380707E+02
FES(L) BAR 73FE 1.S 1. 0. 0.L 1468.000 5000.000
 0.85549011E+01 0.0 0.0 0.0 0.0 0.0
 -0.11493562E+05-0.39585678E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
FES04(S) J 6/66FE 1.S 1.0 4. 0.S 300.000 2000.000
 0.11608929E+02 0.13804697E-01-0.98126384E-05 0.36087811E-08-0.50976280E-12
 -0.11619187E+06-0.56477814E+02 0.35057688E+01 0.37029702E-01-0.29033530E-04
 0.45778599E-08 0.26202087E-11-0.11416250E+06-0.15223241E+02
FES2(S) BAR 73FE 1.S 2. 0. 0.S 300.000 2000.000
 0.20638494E+01 0.29632885E-01-0.48079673E-04 0.35916273E-07-0.10024811E-10
 -0.23009266E+05-0.12381325E+02 0.20638494E+01 0.29632885E-01-0.48079673E-04
 0.35916273E-07-0.10024811E-10-0.23009266E+05-0.12381325E+02
FESIO3(S) J 2/76FE 1.SI 1.0 3. 0.S 298.15 1413.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.25588875E+01 0.25249843E-01-0.11406997E-04
 -0.38646775E-08 0.28174277E-11-0.14528537E+06-0.92577019E+01
FE2CL4 J12/70FE 2.CL 4.0 0.0 0.G 300.000 5000.000
 0.15357500E+02 0.64207870E-03 0.20817730E-07-0.51580559E-10 0.60673478E-14
 -0.56510035E+05-0.31909744E+02 0.12738242E+02 0.13235558E-01-0.21641870E-04
 0.15993667E-07-0.43507099E-11-0.56106578E+05-0.19837906E+02
FE203(S) J 6/65FE 2.0 3.0 0.0 0.S 300.000 2500.000

0.40497528E+02-0.46131596E-01 0.31826406E-04-0.89226333E-08 0.84655416E-12
 -0.11317625E+06-0.21635088E+03-0.77037840E+01 0.13647473E+00-0.32905652E-03
 0.38150478E-06-0.16310285E-09-0.10080075E+06 0.25292084E+02
 FE2S3012 (S) J 6/66FE 2.5 3.0 12. 0.S 300.000 2000.000
 0.39114441E+02 0.11796325E-01-0.33871014E-07-0.22970399E-08 0.64101984E-12
 -0.32478262E+06-0.19400429E+03 0.11116955E+02 0.83706796E-01-0.41365071E-04
 -0.25279220E-07 0.21041432E-10-0.31729781E+06-0.49288757E+02
 FE2SIC4 (S) J 2/76FE 2.SI 1.0 4. 0.S 298.15 1490.0
 0.0 0.0 0.0 0.0
 0.0 0.0 0.18704285E+02 0.15118159E-02 0.21320029E-05
 0.62878236E-09-0.47163776E-12-0.18390319E+06-0.90221283E+02
 FE304 (S) J 6/65FE 3.0 4.0 0.0 0.S 300.000 5000.000
 0.24133713E+02 0.41592226E-04-0.26331492E-07 0.66035094E-11-0.56924680E-15
 -0.14121050E+06-0.12006412E+03 0.36198151E+02-0.17437977E+00 0.52475673E-03
 -0.54238217E-06 0.17996202E-09-0.14138731E+06-0.15556683E+03
 H J 6/74H 1. 0. 0.G 300.000 5000.000
 0.25000000E+01 0.70881145E-09-0.38728927E-12 0.85096609E-16-0.65768064E-20
 0.25474391E+05-0.45989621E+00 0.25000000E+01-0.19925608E-08 0.54929897E-11
 -0.64292206E-14 0.26794034E-17 0.25474391E+05-0.45989943E+00
 H+ J 6/66H 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0
 0.18403344E+06-0.11538620E+01 0.25000000E+01 0.0 0.0
 0.0 0.0 0.18403344E+06-0.11538620E+01
 H- J 9/65H 1.E 1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0
 0.15961047E+05-0.11524487E+01 0.25000000E+01 0.0 0.0
 0.0 0.0 0.15961047E+05-0.11524487E+01
 HALO J 3/64H 1.AL 1.0 1.00 0.G 300.000 5000.000
 0.48556051E+01 0.28598933E-02-0.12152823E-05 0.22966419E-09-0.16047591E-13
 0.21454053E+04-0.32954979E+01 0.18980217E+01 0.77763796E-02 0.15224668E-05
 -0.86530747E-08 0.41700376E-11 0.31156301E+04 0.12763795E+02
 HBO J12/64H 1.B 1.0 1.00 0.G 300.000 5000.000
 0.39902782E+01 0.35116761E-02-0.14167745E-05 0.25804758E-09-0.17539792E-13
 -0.11539402E+05 0.41315740E+00 0.27000637E+01 0.67921393E-02-0.48161182E-05
 0.21375093E-08-0.48790702E-12-0.11132098E+05 0.72359562E+01
 HBO+ J 6/68H 1.B 1.0 1.E -1.G 300.000 5000.000
 0.44547348E+01 0.31428614E-02-0.12961291E-05 0.23975599E-09-0.16390748E-13
 0.16694875E+06-0.60143149E+00 0.29798546E+01 0.61956383E-02-0.29940029E-05
 0.13452306E-09 0.20881907E-12 0.16744444E+06 0.73616123E+01
 HBO2 J12/64H 1.B 1.0 2.00 0.G 300.000 5000.000
 0.47389517E+01 0.47718771E-02-0.18063492E-05 0.31492897E-09-0.20738311E-13
 -0.69248812E+05-0.33346713E-02 0.28707867E+01 0.78862645E-02-0.40736842E-06
 -0.47059032E-08 0.23548897E-11-0.68624125E+05 0.10167320E+02
 HBR J 9/65H 1.BR 1. 0. 0.G 300.000 5000.000
 0.27935801E+01 0.15655926E-02-0.56171064E-06 0.95783145E-10-0.61813991E-14
 -0.52338398E+04 0.76423702E+01 0.36056690E+01-0.59529440E-03 0.65029570E-06
 0.93781227E-09-0.71141850E-12-0.54389453E+04 0.34831772E+01
 HCL J 9/64H 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.27665882E+01 0.14381884E-02-0.46993000E-06 0.73499415E-10-0.43731091E-14
 -0.11917469E+05 0.64583540E+01 0.35248175E+01 0.29984862E-04-0.86221888E-06
 0.20979720E-08-0.98658234E-12-0.12150508E+05 0.23957710E+01
 HCN L12/69H 1.C 1.N 1.0 0.G 300.000 5000.000
 0.37068119E+01 0.33382804E-02-0.11913316E-05 0.19992917E-09-0.12826451E-13
 0.14962637E+05 0.20794907E+01 0.24513559E+01 0.87208375E-02-0.10094203E-04
 0.67255712E-08-0.17626959E-11 0.15213004E+05 0.80830088E+01
 HCO J12/70H 1.C 1.0 1.0 0.G 300.000 5000.000
 0.34738350E+01 0.34370227E-02-0.13632662E-05 0.24928637E-09-0.17044332E-13
 0.39594044E+04 0.60453339E+01 0.38840189E+01-0.82974439E-03 0.77900813E-05
 -0.70616970E-08 0.19971733E-11 0.40563860E+04 0.48354130E+01

HCO+	J12/70H	1.C	1.0	1.E	-1.G	300.000	5000.000
0.37411880E+01	0.33441517E-02	-0.12397122E-05	0.21189388E-09	-0.13704149E-13			
0.98884062E+05	0.20654764E+01	0.24739733E+01	0.86715594E-02	-0.10031500E-04			
0.67170518E-08	-0.17872674E-11	0.99146625E+05	0.81625748E+01				
HCP	J12/69H	1.C	1.P	1.0	0.G	300.000	5000.000
0.44720011E+01	0.26742145E-02	-0.97089560E-06	0.15708386E-09	-0.88457141E-14			
0.18558086E+05	-0.68781352E+00	0.21111135E+01	0.10707665E-01	-0.10801743E-04			
0.49036970E-08	-0.59717249E-12	0.19110211E+05	0.11067474E+02				
HF	J12/68H	1.F	1.0	0.0	0.G	300.000	5000.000
0.30019188E+01	0.69528935E-03	-0.56135178E-07	-0.14767715E-10	0.22140435E-14			
-0.33624996E+05	0.37575865E+01	0.34659719E+01	0.33246865E-03	-0.10063786E-05			
0.12078301E-08	-0.37137269E-12	-0.33821824E+05	0.10758276E+01				
HI	J 9/61H	1.I	1.	0.	0.G	300.000	5000.000
0.29104004E+01	0.15688187E-02	-0.59227631E-06	0.10537093E-09	-0.70375123E-14			
0.22508660E+04	0.78513079E+01	0.36963720E+01	-0.14224756E-02	0.30131187E-05			
-0.12666403E-08	-0.35098765E-13	0.21073582E+04	0.40749578E+01				
HNCO	J12/70H	1.N	1.C	1.0	1.G	300.000	5000.000
0.51300392E+01	0.43551363E-02	-0.16269023E-05	0.28035596E-09	-0.18276037E-13			
-0.14101785E+05	-0.22010994E+01	0.23722162E+01	0.13664041E-01	-0.13323158E-04			
0.64475465E-08	-0.10402894E-11	-0.13437059E+05	0.11588263E+02				
HNO	J 3/63H	1.N	1.0	1.0	0.G	300.000	5000.000
0.35548620E+01	0.32713183E-02	-0.12734072E-05	0.22602047E-09	-0.15064827E-13			
0.10693734E+05	0.51684904E+01	0.37412004E+01	-0.20067061E-03	0.75409298E-05			
-0.79105718E-08	-0.25928391E-11	0.10817844E+05	0.50063477E+01				
HN02	J 6/63H	1.N	1.0	2.	0.G	300.000	5000.000
0.55144939E+01	0.41394420E-02	-0.15878704E-05	0.27977642E-09	-0.18584208E-13			
-0.11276887E+05	-0.31425257E+01	0.25098877E+01	0.12171604E-01	-0.78618377E-05			
0.35351566E-09	-0.11540855E-11	-0.10450008E+05	0.12399634E+02				
HN03	J 6/63H	1.N	1.0	3.	0.G	300.000	5000.000
0.70591097E+01	0.56769438E-02	-0.22348859E-05	0.40155523E-09	-0.27080511E-13			
-0.18920008E+05	-0.10778285E+02	0.14377136E+01	0.20903554E-01	-0.14574553E-04			
0.11972023E-08	-0.19117286E-11	-0.17385367E+05	0.18246246E+02				
HOF	J12/72H	1.0	1.F	1.	0.G	300.000	5000.000
0.40464334E+01	0.24486282E-02	-0.86283552E-06	0.14209904E-09	-0.89356928E-14			
-0.13209066E+05	0.33367682E+01	0.32310925E+01	0.37389856E-02	0.63009765E-06			
-0.36215002E-08	-0.17867131E-11	-0.12954777E+05	0.77377386E+01				
H02	J 3/64H	1.0	2.00	0.00	0.G	300.000	5000.000
0.37866278E+01	0.27885404E-02	-0.10168706E-05	0.17183946E-09	-0.11021854E-13			
0.11888501E+04	0.48147612E+01	0.35094852E+01	0.11499671E-02	0.58784262E-05			
-0.77795512E-08	-0.29607887E-11	0.13803330E+04	0.68276329E+01				
HS03F	J 6/72H	1.S	1.0	3.F	1.G	300.000	5000.000
0.10364190E+02	0.53861178E-02	-0.21231572E-05	0.38208348E-09	-0.25807092E-13			
-0.94398312E+05	-0.26018753E+02	0.21192446E+01	0.31545710E-01	-0.31317890E-04			
0.12461506E-07	-0.82514632E-12	-0.92361625E+05	0.15546442E+02				
H2	J 3/61H	2.0	0.0	0.0	0.G	300.000	5000.000
0.31001902E+01	0.51119458E-03	0.52644211E-07	-0.34909978E-10	0.36945341E-14			
-0.87738037E+03	-0.19629421E+01	0.30574455E+01	0.26765200E-02	-0.58099158E-05			
0.55210378E-08	-0.18122743E-11	-0.98890479E+03	-0.22997055E+01				
H20 (S)	L11/65H	2.0	1.00	0.00	0.S	200.000	273.150
0.0	0.0	0.0	0.0	0.0	0.0		
0.0	0.0	-0.39269332E-01	0.16920421E-01	0.0			
0.0	0.0	-0.35949582E+05	0.56933784E+00				
H20 (L)	L11/65H	2.0	1.00	0.00	0.L	273.150	1000.000
0.0	0.0	0.0	0.0	0.0	0.0		
0.0	0.0	0.12712782E+02	-0.17662790E-01	-0.22556662E-04			
0.20820909E-06	-0.24078606E-09	-0.37483199E+05	-0.59115341E+02				
H20	J 3/61H	2.0	1.00	0.00	0.G	300.000	5000.000
0.27167635E+01	0.29451374E-02	-0.80224373E-06	0.10226682E-09	-0.48472138E-14			
-0.29905824E+05	0.66305676E+01	0.40701275E+01	-0.11084499E-02	0.41521180E-05			

-0.29637404E-08 0.80702101E-12-0.30279723E+05-0.32270044E+00
 H202 L 2/69H 2.0 2.0 0.0 0.G 300.000 5000.000
 0.45731668E+01 0.43361373E-02-0.14746884E-05 0.23489033E-09-0.14316537E-13
 -0.18006961E+05 0.50113696E+00 0.33887539E+01 0.65692253E-02-0.14850127E-06
 -0.46258037E-08 0.24715143E-11-0.17663148E+05 0.67853632E+01
 H2S J12/65H 2.S 1.00 0.00 0.G 300.000 5000.000
 0.28479099E+01 0.38415990E-02-0.14099369E-05 0.24278757E-09-0.15783283E-13
 -0.34469788E+04 0.74781408E+01 0.38811293E+01-0.13211856E-03 0.36517722E-05
 -0.21820445E-08 0.28783779E-12-0.36350918E+04 0.25161514E+01
 H2S04 (L) J12/66H 2.S 1.0 4. 0.L 300.000 2000.000
 0.19537796E+02 0.22764318E-02-0.46662656E-08-0.83314866E-09 0.24879729E-12
 -0.10441887E+06-0.94525696E+02 0.64979801E+01 0.52939959E-01-0.76283832E-04
 0.51075961E-07-0.13004852E-10-0.10161100E+06-0.30963394E+02
 H2S04 J12/66H 2.S 1.0 4. 0.G 300.000 5000.000
 0.10893733E+02 0.73577948E-02-0.27934020E-05 0.48889848E-09-0.32326918E-13
 -0.93185875E+05-0.30424438E+02 0.10093718E+01 0.39770886E-01-0.40434359E-04
 0.17110583E-07-0.15417849E-11-0.90814562E+05 0.19098511E+02
 H3B306 J12/64H 3.B 3.0 6.00 0.G 300.000 5000.000
 0.20153580E+02 0.13016287E-01-0.50669623E-05 0.90308250E-09-0.60532417E-13
 -0.28104094E+06-0.79689529E+02-0.22705116E+01 0.87024868E-01-0.91587717E-04
 0.39445393E-07-0.36666035E-11-0.27569525E+06 0.32516449E+02
 HE L 5/66HE 1.00 0.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0
 -0.74537500E+03 0.91534889E+00 0.25000000E+01 0.0 0.0
 0.0 0.0 -0.74537500E+03 0.91534883E+00
 HE+ L12/66HE 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0
 0.28534269E+06 0.16084042E+01 0.25000000E+01 0.0 0.0
 0.0 0.0 0.28534269E+06 0.16084042E+01
 HG(L) J12/61HG 1. 0. 0. 0.L 300.000 5000.000
 0.30456257E+01 0.31731301E-03 0.38948308E-07-0.99941748E-11 0.87930660E-15
 -0.89334448E+03-0.82292366E+01 0.37440119E+01-0.17082968E-02 0.12534801E-05
 0.92447539E-09-0.82090698E-12-0.10530312E+04-0.11741219E+02
 HG J12/61HG 1. 0. 0. 0.G 300.000 5000.000
 0.24891195E+01 0.20372856E-04-0.11934368E-07 0.26220554E-11-0.18015364E-15
 0.66319922E+04 0.68468409E+01 0.25204592E+01-0.14275590E-03 0.34869095E-06
 -0.35726133E-09 0.13086765E-12 0.66257695E+04 0.67003660E+01
 HGBR2(S) J 3/62HG 1.BR 2. 0. 0.S 300.000 514.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.82829714E+01 0.16302364E-02 0.34229879E-05
 0.70961992E-09-0.43353862E-11-0.22952437E+05-0.27345276E+02
 HGBR2(L) J 3/62HG 1.BR 2. 0. 0.L 514.000 5000.000
 0.12278799E+02 0.0 0.0 0.0 0.0
 -0.22500898E+05-0.46851212E+02 0.12278799E+02 0.0 0.0
 0.0 0.0 -0.22500898E+05-0.46851212E+02
 HGBR2 J 3/62HG 1.BR 2. 0. 0.G 300.000 5000.000
 0.74226990E+01 0.78687663E-04-0.29910307E-07 0.48498228E-11-0.27930933E-15
 -0.12522020E+05-0.38805027E+01 0.67188921E+01 0.25782743E-02-0.29180237E-05
 0.95818442E-09 0.13872307E-12-0.12371434E+05-0.42683381E+00
 HGO(S) J 6/62HG 1.0 1. 0. 0.S 300.000 1000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.34170866E+01 0.71160570E-02-0.14896996E-05
 -0.44913548E-08 0.25937924E-11-0.12233270E+05-0.13037185E+02
 I J 6/74I 1. 0. 0. 0.G 300.000 5000.000
 0.26527205E+01-0.33767940E-03 0.23257491E-06-0.50119353E-10 0.35652227E-14
 0.12046039E+05 0.66688499E+01 0.25005808E+01-0.59243166E-05 0.21150878E-07
 -0.31604885E-10 0.16858974E-13 0.12095488E+05 0.74842529E+01
 I2(S) J 9/61I 2. 0. 0. 0.S 300.000 386.750
 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.59920378E+01-0.77115069E-03 0.30346155E-05
 0.99078390E-09 0.61171873E-10-0.18097739E+04-0.20206406E+02
 I2(L) J 9/61I 2. 0. 0. 0.L 386.750 5000.000
 0.97027674E+01 0.0 0.0 0.0 0.0 0.0
 -0.12663264E+04-0.37198486E+02 0.97027674E+01 0.0 0.0
 0.0 0.0 -0.12663264E+04-0.37198486E+02
 I2 J 9/61I 2. 0. 0. 0.G 300.000 5000.000
 0.44710817E+01 0.10020430E-03-0.14380571E-07 0.27741941E-11-0.19669640E-15
 0.61639531E+04 0.58150349E+01 0.41670017E+01 0.14456720E-02-0.22818413E-05
 0.17076469E-08-0.47899532E-12 0.62206602E+04 0.72552214E+01
 IR(S) H11/76IR 1.0 0.0 0.0 0.S 298.150 2716.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.11670616E+02 0.16638961E-01-0.31867212E-05
 -0.12665211E-08 0.37552719E-12 0.75743477E+04 0.74056824E+02
 IR H11/76IR 1.0 0.0 0.0 0.G 298.150 5000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.14841576E+01 0.17372093E-02-0.50628688E-06
 0.65155381E-10-0.29331910E-14 0.80188750E+05 0.14659647E+02
 K(S) J12/61K 1.0 0.0 0.0 0.S 300.000 336.350
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.17263231E+01-0.98042772E-04 0.13852978E-04
 0.57915802E-07-0.11734935E-09-0.69166992E+03-0.29234371E+01
 K(L) J12/61K 1.0 0.0 0.0 0.L 336.350 2000.000
 0.32625046E+01-0.13113792E-03 0.50811991E-06 0.62810507E-10-0.51130459E-13
 -0.52525244E+03-0.96002321E+01 0.44202108E+01-0.19475967E-02 0.61695016E-06
 0.89816043E-09-0.33655804E-12-0.96275781E+03-0.16042435E+02
 K J 6/62K 1.00 0.00 0.00 0.G 300.000 5000.000
 0.25673647E+01-0.14933596E-03 0.12342446E-06-0.53394233E-10 0.11948426E-13
 0.99550547E+04 0.46642084E+01 0.24930964E+01 0.50164177E-04-0.12751224E-06
 0.13540491E-09-0.51145936E-13 0.99786367E+04 0.50560436E+01
 K+ J 3/65K 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0 0.0
 0.61096559E+05 0.43339453E+01 0.25000000E+01 0.0 0.0 0.0
 0.0 0.0 0.61096559E+05 0.43339453E+01
 KALO2(L) CH3/77K 1.AL 1.0 2.0 0.L 300.000 3600.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.59992493E+02-0.40612478E-01 0.85234014E-05
 0.10477745E-08-0.33993034E-12-0.18309700E+06-0.35413721E+03
 KALSI04(L) CH3/77K 1.AL 1.SI 1.0 4.L 300.000 3600.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.23478851E+02-0.58577070E-03 0.33144840E-06
 -0.81825713E-10 0.74460938E-14-0.24304544E+06-0.11351299E+03
 KALSI206(L) CH3/77K 1.AL 1.SI 2.0 6.L 300.000 3600.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.33210892E+02-0.13323724E-02 0.75273368E-06
 -0.18548045E-09 0.16842905E-13-0.34319650E+06-0.15832576E+03
 KALSI308(S) GS4/76K 1.AL 1.SI 3.0 8.S 298.15 1400.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.25785995E+02 0.18233709E-01-0.16221438E-05
 -0.79023117E-08 0.35324920E-11-0.48505737E+06-0.12652226E+03
 KALSI308(L) CH3/77K 1.AL 1.SI 3.0 8.L 1400.000 3600.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.48245926E+02-0.31747145E-02 0.11813618E-05
 -0.16981620E-09 0.64346823E-14-0.49460194E+06-0.26058862E+03
 KBC2 J 6/71K 1.B 1.0 2.0 0.G 300.000 5000.000
 0.75502510E+01 0.25661823E-02-0.10671565E-05 0.19851885E-09-0.13704166E-13
 -0.83653812E+05-0.85058813E+01 0.43967800E+01 0.12169201E-01-0.11804218E-04
 0.51316533E-08-0.65932719E-12-0.82827000E+05 0.75600615E+01
 KCL(S) J 3/66K 1.CI 1.00 0.00 0.S 300.000 1044.000

0.39157171E+01-0.20927270E-02 0.47310186E-05 0.70152524E-08-0.55146096E-11
 -0.52747066E+05-0.10144800E+02 0.53934307E+01 0.26535243E-02 0.96075655E-06
 -0.50251856E-08 0.40721228E-11-0.54248391E+05-0.21596817E+02
 KCL(L) J 3/66K 1.CL 1.00 0.00 O.L 1044.000 5000.000
 0.88518066E+01 0.0 0.0 0.0 0.0
 -0.53369477E+05-0.40010056E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 KCL J 3/66K 1.CL 1.00 0.00 O.G 300.000 5000.000
 0.44636736E+01 0.12229207E-03-0.91719201E-08 0.92648285E-12-0.10407917E-16
 -0.27173133E+05 0.32349329E+01 0.39908571E+01 0.21089169E-02-0.31836526E-05
 0.22525308E-08-0.59094179E-12-0.27080184E+05 0.54988480E+01
 KF(S) J 6/69K 1.F 1.0 0.0 O.S 300.000 1131.000
 0.94627781E+01-0.64057522E-02 0.63913262E-07 0.75949593E-08-0.33598107E-11
 -0.71249125E+05-0.44831802E+02 0.49843969E+01 0.35943191E-02-0.17696402E-05
 -0.48106141E-09 0.10280726E-11-0.70018125E+05-0.21384506E+02
 KF(L) J 6/69K 1.F 1.0 0.0 O.L 1131.000 5000.000
 0.86555471E+01 0.0 0.0 0.0 0.0
 -0.69268000E+05-0.41179932E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 KF J 6/69K 1.F 1.0 0.0 O.G 300.000 5000.000
 0.44040699E+01 0.17833726E-03-0.36093798E-07 0.58839591E-11-0.34694046E-15
 -0.40655891E+05 0.20179329E+01 0.35156069E+01 0.37868421E-02-0.55864994E-05
 0.37751455E-08-0.93924261E-12-0.40476078E+05 0.63002224E+01
 KF2- J12/68K 1.F 2.E 1.0 O.G 300.000 5000.000
 0.72581635E+01 0.26703556E-03-0.11384628E-06 0.21407681E-10-0.14827070E-14
 -0.85780812E+05-0.10116452E+02 0.52507572E+01 0.86383708E-02-0.13403673E-04
 0.94140837E-08-0.24682600E-11-0.85384000E+05-0.49039841E+00
 KHF2(S) J 6/71K 1.H 1.F 2.0 O.S 300.000 469.850
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.91298494E+01 0.86618900E-01 0.43904409E-04
 -0.66867597E-06 0.80454154E-09-0.11258256E+06 0.41082794E+02
 KHF2(S) J 6/71K 1.H 1.F 2.0 O.S 469.850 511.950
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.12057378E+02 0.0 0.0
 0.0 0.0 -0.11457125E+06-0.54170135E+02
 KHF2(L) J 6/71K 1.H 1.F 2.0 O.L 511.950 6000.000
 0.12580737E+02 0.0 0.0 0.0 0.0
 -0.11404306E+06-0.55879913E+02 0.12580737E+02 0.0 0.0
 0.0 0.0 -0.11404306E+06-0.55879913E+02
 K2F2 J 6/69K 2.F 2.0 0.0 O.G 300.000 5000.000
 0.98148098E+01 0.20453081E-03-0.87071669E-07 0.16337223E-10-0.11287256E-14
 -0.10675987E+06-0.17654968E+02 0.78329506E+01 0.89240819E-02-0.14719852E-04
 0.10982468E-07-0.30721719E-11-0.10638750E+06-0.82555456E+01
 KO J12/67K 1.0 1. 0. O.G 300.000 5000.000
 0.44244776E+01 0.19936154E-03-0.37128839E-07 0.71308298E-11-0.50369682E-15
 0.72052344E+04 0.32945051E+01 0.37410774E+01 0.31242017E-02-0.48020038E-05
 0.34660605E-08-0.93599781E-12 0.73368711E+04 0.65537605E+01
 KC- J12/67K 1.0 1.E 1. O.G 300.000 5000.000
 0.44201088E+01 0.20124266E-03-0.39330995E-07 0.75598512E-11-0.53442273E-15
 -0.17956109E+05 0.19068260E+01 0.37083664E+01 0.32376479E-02-0.49690498E-05
 0.35728847E-08-0.96080262E-12-0.17818605E+05 0.53034477E+01
 KOH(S) J12/70K 1.0 1.H 1.0 O.S 300.000 516.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.64400978E+01 0.11310168E-02 0.15073272E-04
 -0.14906117E-07 0.10556325E-10-0.53161898E+05-0.28098846E+02
 KOH(S) J12/70K 1.0 1.H 1.0 O.S 516.000 679.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.94607143E+01 0.0 0.0
 0.0 0.0 -0.53291648E+05-0.43369324E+02

KOH(L) J12/70K 1.0 1.H 1.0 0.L 679.000 5000.000
 0.99956465E+01 0.0 0.0 0.0 0.0 0.0
 -0.52620730E+05-0.45334396E+02 0.99956465E+01 0.0 0.0
 0.0 0.0 -0.52620730E+05-0.45334396E+02
 KOH J12/70K 1.0 1.H 1.0 0.G 300.000 5000.000
 0.56400948E+01 0.12510226E-02-0.34984549E-06 0.44566989E-10-0.20870280E-14
 -0.29698730E+05-0.40568190E+01 0.40733442E+01 0.97217932E-02-0.15988800E-04
 0.12148352E-07-0.33709346E-11-0.29506559E+05 0.29222374E+01
 KOH+ J12/71K 1.0 1.H 1.E -1.G 300.000 5000.000
 0.56806145E+01 0.12120951E-02-0.33447117E-06 0.41727927E-10-0.18793912E-14
 0.58167602E+05-0.25673008E+01 0.44325171E+01 0.84631629E-02-0.14247855E-04
 0.11106625E-07-0.31563615E-11 0.58292633E+05 0.28601961E+01
 K2 J12/61K 2.00 0.00 0.00 0.G 300.000 5000.000
 0.45089998E+01 0.22596406E-03 0.14957173E-07-0.38811532E-11 0.34052376E-15
 0.13926066E+05 0.42568560E+01 0.44424906E+01 0.46158722E-03-0.30025598E-06
 0.17502910E-09-0.32470554E-13 0.13941672E+05 0.45868359E+01
 K2C03(S) J 3/66K 2.C 1.0 3. 0.S 300.000 1174.000
 0.22824341E+02-0.13580993E-01 0.87409890E-05 0.11494425E-07-0.67588149E-11
 -0.14577844E+06-0.11048665E+03 0.84398632E+01 0.18836256E-01-0.46827483E-06
 -0.10519610E-07 0.64318412E-11-0.14166744E+06-0.34894424E+02
 K2C03(L) J 3/66K 2.C 1.0 3. 0.L 1174.000 5000.000
 0.25161469E+02 0.0 0.0 0.0 0.0 0.0
 -0.14740137E+06-0.13110730E+03 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 K2O(S) J 6/63K 2.0 1.00 0.00 0.S 300.000 2000.000
 0.86890736E+01 0.51097497E-02-0.20386506E-06 0.58747271E-10-0.10899823E-14
 -0.46449234E+05-0.39589233E+02 0.34449682E+01 0.40567029E-01-0.82051687E-04
 0.79006099E-07-0.27313776E-10-0.45925457E+05-0.17385208E+02
 K2O(L) CH3/77K 2.0 1.0 0.0 0.L 2000.000 3600.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.87453308E+01 0.15975829E-01-0.22929680E-05
 -0.62914962E-09 0.13636417E-12-0.25041918E+05 0.78889404E+02
 K2S04(S) J12/71K 2.S 1.0 4. 0.S 300.000 857.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.86070185E+01 0.16985351E+00-0.42177970E-03
 0.48328019E-06-0.19513494E-09-0.17500300E+06 0.34369980E+02
 K2S04(S) J12/71K 2.S 1.0 4. 0.S 857.000 1342.000
 -0.60829883E+03 0.11671629E+01-0.19272040E-03-0.64296722E-06 0.29993918E-09
 0.31675883E+05 0.33161084E+04-0.17481522E+02 0.38860269E-01 0.38084880E-04
 -0.16443334E-07-0.19904162E-10-0.16458725E+06 0.11890733E+03
 K2S04(L) J 7/77K 2.S 1.0 4. 0.L 1342.00 3000.000
 0.23852859E+02-0.42390800E-03 0.36037449E-06-0.12888612E-09 0.16487002E-13
 -0.17594694E+06-0.11413211E+03 0.12225206E+02 0.14974866E-01-0.23317320E-04
 0.62640140E-07-0.42845963E-10-0.17124581E+06-0.47578369E+02
 K2SC4 IJ4/76K 2.S 1.0 4. 0.G 300.00 3000.00
 0.15430134E+02 0.39032621E-02-0.15048181E-05 0.18303541E-09 0.44845007E-14
 -0.13656044E+06-0.44412979E+02 0.61823664E+01 0.31592138E-01-0.27527392E-04
 0.50265037E-08 0.27424885E-11-0.13424137E+06 0.24917498E+01
 K202H2 J12/70K 2.0 2.H 2.0 0.G 300.000 5000.000
 0.95097723E+01 0.54167062E-02-0.19223535E-05 0.31866065E-09-0.20152510E-13
 -0.82048375E+05-0.16825668E+02 0.69190598E+01 0.10300703E-01-0.25173296E-06
 -0.77450011E-08 0.40796038E-11-0.81260562E+05-0.29860201E+01
 K2SiO3(S) J 4/76K 2.SI 1.0 3.0 0.S 298.15 1249.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.99588022E+01 0.19306805E-01-0.43248729E-05
 -0.69299908E-08 0.35243648E-11-0.19005150E+06-0.44897339E+02
 K2SiO3(L) J 4/76K 2.SI 1.0 3.0 0.L 1249.00 3000.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.21249054E+02 0.17914608E-03 0.16543532E-06

-0.11645357E-09 0.18639170E-13-0.18809837E+06-0.10244969E+03
 K2SI2C5(L) PB7/77K 2.SI 2.0 5.0 0.L 300.00 3600.000
 0.41488983E+02-0.15134875E-01 0.90504391E-05-0.23028943E-08 0.21212367E-12
 -0.30808394E+06-0.21548285E+03 0.75679197E+01 0.76197922E-01-0.17800601E-03
 0.25759209E-06-0.13003822E-09-0.29640081E+06-0.33038101E+02
 LI(S) J 6/62LI 1.0 0.0 0.0 0.S 300.000 453.690
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.91818619E+01-0.35999309E-01 0.24881856E-05
 0.26456524E-06-0.34331049E-09-0.15189534E+04-0.39845856E+02
 LI(L) J 6/62LI 1.0 0.0 0.0 0.L 453.690 4000.000
 0.36114159E+01-0.18325284E-03 0.40743757E-07 0.26515630E-11-0.11572503E-14
 -0.74925732E+03-0.16352737E+02 0.38988094E+01 0.61335438E-03-0.48307647E-05
 0.61290351E-08-0.23400344E-11-0.87493872E+03-0.18156235E+02
 LI J 6/62LI 1.00 0.00 0.00 0.G 300.000 5000.000
 0.24737692E+01 0.87435343E-04-0.90773597E-07 0.31327926E-10-0.17579908E-14
 0.18588035E+05 0.25630283E+01 0.25103741E+01-0.74235737E-04 0.18612565E-06
 -0.19540847E-09 0.73145266E-13 0.18581672E+05 0.23902454E+01
 LI+ J 3/65LI 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0 0.0
 0.81899062E+05 0.17406168E+01 0.25000000E+01 0.0 0.0
 0.0 0.0 0.81899062E+05 0.17406168E+01
 LIBC2 J 6/71LI 1.B 1.0 2.0 0.G 300.000 5000.000
 0.74266100E+01 0.27043757E-02-0.11284737E-05 0.21062398E-09-0.14584908E-13
 -0.80370312E+05-0.10613985E+02 0.37435474E+01 0.14475256E-01-0.15209688E-04
 0.74136537E-08-0.12242195E-11-0.79437750E+05 0.79988327E+01
 LICL(S) J 6/62LI 1.CL 1.00 0.00 0.S 300.000 883.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.41095247E+01 0.81981011E-02-0.11541874E-04
 0.10585385E-07-0.36457018E-11-0.50608266E+05-0.18298889E+02
 LICL(L) J 6/62LI 1.CL 1.00 0.00 0.L 883.000 2000.000
 0.82149477E+01 0.56391372E-03-0.17350330E-05 0.76594997E-09-0.12378477E-12
 -0.50007320E+05-0.38808960E+02 0.10383028E+02-0.47179684E-02-0.16138320E-05
 0.80807183E-08-0.44459497E-11-0.50539121E+05-0.49921967E+02
 LICL J 6/62LI 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.42712145E+01 0.31400286E-03-0.10123131E-06 0.18451851E-10-0.12398731E-14
 -0.24884441E+05 0.10285692E+01 0.29906902E+01 0.50338656E-02-0.65671975E-05
 0.38050167E-08-0.76117454E-12-0.24603184E+05 0.73150320E+01
 LIF(S) J12/68LI 1.F 1.0 0.0 0.S 300.000 1121.300
 0.55405741E+01-0.13421080E-03 0.17825605E-05 0.88996455E-09-0.91296675E-12
 -0.75900375E+05-0.27447281E+02 0.17694321E+01 0.17505225E-01-0.28038747E-04
 0.22893385E-07-0.69633656E-11-0.75299250E+05-0.99478054E+01
 LIF(L) J12/68LI 1.F 1.0 0.0 0.L 1121.300 5000.000
 0.77195396E+01 0.0 0.0 0.0 0.0 0.0
 -0.74304375E+05-0.38815491E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 LIF J12/68LI 1.F 1.0 0.0 0.G 300.000 5000.000
 0.40430250E+01 0.57041063E-03-0.21454144E-06 0.40609016E-10-0.28357920E-14
 -0.42299316E+05 0.68453211E+00 0.28528872E+01 0.39532781E-02-0.31724985E-05
 0.43244408E-09 0.37055667E-12-0.41987266E+05 0.67778654E+01
 LIF2- J12/68LI 1.F 2.E 1.0 0.G 300.000 5000.000
 0.63448591E+01 0.12571272E-02-0.53522831E-06 0.10113024E-09-0.70581731E-14
 -0.87667875E+05-0.93115845E+01 0.34718132E+01 0.10636713E-01-0.11777646E-04
 0.56765472E-08-0.84659840E-12-0.86963125E+05 0.51277466E+01
 LIFC J 9/65LI 1.F 1.0 1.00 0.G 300.000 5000.000
 0.59926109E+01 0.11139200E-02-0.47888494E-06 0.91068333E-10-0.63849106E-14
 -0.13100988E+05-0.53497667E+01 0.25001793E+01 0.12661718E-01-0.14157589E-04
 0.64506374E-08-0.74261430E-12-0.12265535E+05 0.12130855E+02
 LIH(S) J 9/67LI 1.H 1.00 0.00 0.S 300.000 961.800
 0.0 0.0 0.0 0.0 0.0 0.0

0.0 0.0 0.38611811E+00 0.12127958E-01-0.86900336E-05
 0.56311542E-08-0.12693483E-11-0.11486992E+05-0.30654573E+01
 LIH(L) J 9/67LI 1.H 1.00 0.00 0.L 961.800 5000.000
 0.74981194E+01 0.0 0.0 0.0 0.0 0.0
 -0.11581824E+05-0.40047272E+02 0.74981194E+01 0.0 0.0
 0.0 0.0 -0.11581824E+05-0.40047272E+02
 LIH J 9/67LI 1.H 1.00 0.00 0.G 300.000 5000.000
 0.35884295E+01 0.10727691E-02-0.40194590E-06 0.73828554E-10-0.49269636E-14
 0.15717625E+05-0.38820952E+00 0.34209490E+01-0.68067363E-03 0.56527379E-05
 -0.62180341E-08 0.21531752E-11 0.15884945E+05 0.10525713E+01
 LIN J12/66LI 1.N 1.00 0.00 0.G 300.000 5000.000
 0.42258081E+01 0.39667194E-03-0.12493990E-06 0.23174754E-10-0.15851917E-14
 0.38916953E+05 0.68768561E+00 0.28894300E+01 0.52212551E-02-0.65969025E-05
 0.37288999E-08-0.72355143E-12 0.39216324E+05 0.72757053E+01
 LIO J 3/64LI 1.O 1.00 0.00 0.G 300.000 5000.000
 0.41876202E+01 0.41186577E-03-0.14520293E-06 0.27253075E-10-0.18864775E-14
 0.87795273E+04 0.12182627E+01 0.28389006E+01 0.51538609E-02-0.63082380E-05
 0.34114385E-08-0.61631342E-12 0.90884297E+04 0.78999548E+01
 LIO- J12/67LI 1.O 1.E 1.0 0.G 300.000 5000.000
 0.41810217E+01 0.41784998E-03-0.15024847E-06 0.28397729E-10-0.19789182E-14
 -0.93849687E+04-0.15559107E+00 0.28515863E+01 0.50169863E-02-0.59547474E-05
 0.30399452E-08-0.47872969E-12-0.90778086E+04 0.64462719E+01
 LIOH(S) J 6/71LI 1.O 1.H 1.0 0.S 300.000 744.300
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.63227797E+00 0.25340538E-01-0.27897957E-04
 0.86925880E-08 0.41499894E-11-0.59412680E+05-0.48382692E+01
 LIOH(L) J 6/71LI 1.O 1.H 1.0 0.L 744.300 5000.000
 0.10474218E+02 0.0 0.0 0.0 0.0 0.0
 -0.60185672E+05-0.53897141E+02 0.10474218E+02 0.0 0.0
 0.0 0.0 -0.60185672E+05-0.53897141E+02
 LIOH J 6/71LI 1.O 1.H 1.0 0.G 300.000 5000.000
 0.55096960E+01 0.13685464E-02-0.39441471E-06 0.52332194E-10-0.25958676E-14
 -0.29899230E+05-0.65201817E+01 0.33462296E+01 0.11787254E-01-0.18252656E-04
 0.13085614E-07-0.34328738E-11-0.29564637E+05 0.34480677E+01
 LIOH+ J12/71LI 1.O 1.H 1.E -1.G 300.000 5000.000
 0.55329266E+01 0.13777930E-02-0.40659307E-06 0.55590907E-10-0.28604625E-14
 0.91888562E+05-0.50067244E+01 0.36379738E+01 0.10897156E-01-0.17229671E-04
 0.12667925E-07-0.34165257E-11 0.92161187E+05 0.36246300E+01
 LION J 9/66LI 1.O 1.N 1.00 0.G 300.000 5000.000
 0.58123493E+01 0.12870627E-02-0.54667709E-06 0.10314986E-09-0.71930444E-14
 0.19692301E+05-0.43578701E+01 0.36701164E+01 0.72568171E-02-0.58681144E-05
 0.11628312E-08 0.42704121E-12 0.202711703E+05 0.66693306E+01
 LI2 J 6/62LI 2.00 0.00 0.00 0.G 300.000 5000.000
 0.44338760E+01 0.22848941E-03-0.24519025E-07 0.39448817E-11-0.22839502E-15
 0.24005746E+05-0.17116909E+01 0.37418919E+01 0.31246294E-02-0.46337063E-05
 0.32618304E-08-0.85308214E-12 0.24142156E+05 0.16040726E+01
 LI2CL2 J 6/62LI 2.CL 2.00 0.00 0.G 300.000 5000.000
 0.95245609E+01 0.52458839E-03-0.22337952E-06 0.41951109E-10-0.29021305E-14
 -0.74990250E+05-0.20044830E+02 0.52801352E+01 0.18384099E-01-0.28769442E-04
 0.20313358E-07-0.53433247E-11-0.74160000E+05 0.26612705E+00
 LI2F2 J12/68LI 2.F 2.0 0.0 0.G 300.000 5000.000
 0.89566631E+01 0.11719270E-02-0.50990502E-06 0.97917535E-10-0.69215602E-14
 -0.11637225E+06-0.20899490E+02 0.24007511E+01 0.27066238E-01-0.39256178E-04
 0.25722599E-07-0.62237229E-11-0.11501094E+06 0.10878616E+02
 LI2O(S) J 3/64LI 2.O 1.00 0.00 0.S 300.000 1843.000
 0.42774773E+01 0.78521669E-02-0.52225090E-06-0.17864425E-08 0.53961035E-12
 -0.73396250E+05-0.21765503E+02-0.31727237E+00 0.36149357E-01-0.55455923E-04
 0.41796437E-07-0.11804048E-10-0.73106187E+05-0.22888327E+01
 LI2O(L) J 3/64LI 2.O 1.00 0.00 0.L 1843.000 5000.000

C.12076931E+02	0.0	0.0	0.0	0.0
-0.71337937E+05	-0.65174973E+02	0.0	0.0	0.0
0.0	0.0	0.0	0.0	
LI20	J 3/64LI	2.0	1.00 0.00 0.G	300.000 5000.000
0.66198750E+01	0.96879457E-03	-0.41490506E-06	0.78637333E-10	-0.54969287E-14
-0.22255324E+05	-0.10834722E+02	0.39721708E+01	0.92460923E-02	-0.93596145E-05
0.34639160E-08	-0.75658880E-13	-0.21596988E+05	0.25391407E+01	
LI202	J 3/64LI	2.0	2.00 0.00 0.G	300.000 5000.000
0.95275259E+01	0.53021009E-03	-0.23005862E-06	0.44030835E-10	-0.31018702E-14
-0.32182484E+05	-0.21872269E+02	0.55375233E+01	0.17344221E-01	-0.27197966E-04
0.19305627E-07	-0.51207953E-11	-0.31402043E+05	-0.27814760E+01	
LI202H2	J 6/71LI	2.C	2.H 2.0 0.G	300.000 5000.000
0.89936132E+01	0.60039647E-02	-0.21810183E-05	0.36888737E-09	-0.23738014E-13
-0.88844125E+05	-0.21371811E+02	0.28646641E+01	0.25237311E-01	-0.22632797E-04
0.74632709E-08	0.22925498E-12	-0.87338812E+05	0.95299644E+01	
LI3CL3	J 6/62LI	3.CL	3.00 0.00 0.G	300.000 5000.000
0.14319440E+02	0.18854006E-02	-0.81978328E-06	0.15735493E-09	-0.11119472E-13
-0.12558850E+06	-0.42724182E+02	0.45745955E+01	0.39749239E-01	-0.56508215E-04
0.36294146E-07	-0.85784704E-11	-0.12353350E+06	0.46674442E+01	
LI3F3	J12/68LI	3.F	3.0 0.0 0.G	300.000 5000.000
0.14364422E+02	0.18285499E-02	-0.79221161E-06	0.15154529E-09	-0.10675675E-13
-0.18723737E+06	-0.45074081E+02	0.46413975E+01	0.39878696E-01	-0.57248995E-04
0.37193544E-07	-0.89230125E-11	-0.18519850E+06	0.21491966E+01	
MG(S)	J 9/62MG	1.0	0.0 0.0 0.S	300.000 922.000
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.20184774E+01	0.52825734E-02	-0.89160058E-05
0.81194536E-08	-0.23538706E-11	-0.77246704E+03	-0.88131208E+01	
MG(L)	J 9/62MG	1.0	0.0 0.0 0.L	922.000 5000.000
0.26570520E+01	0.13083967E-02	0.0	0.0	0.0
0.22868300E+03	-0.10433817E+02	0.26570520E+01	0.13083967E-02	0.0
0.0	0.0	0.22868300E+03	-0.10433817E+02	
MG	J 9/62MG	1.00	0.00 0.00 0.G	300.000 5000.000
0.24188604E+01	0.16145770E-03	-0.99399188E-07	0.18989310E-10	0.91656165E-16
0.17036992E+05	0.40641127E+01	0.24988747E+01	0.87608205E-05	-0.23614632E-07
0.26287528E-10	-0.10308811E-13	0.17008320E+05	0.36263638E+01	
MG+	J12/70MG	1.E	-1.0 0.0 0.G	300.000 5000.000
0.25088720E+01	-0.18270206E-04	0.12600442E-07	-0.35595442E-11	0.35772827E-15
0.10648319E+06	0.42663994E+01	0.24961672E+01	0.27410788E-04	-0.68663780E-07
0.72015616E-10	-0.26930064E-13	0.10648669E+06	0.43307381E+01	
MGBR2(S)	J 6/74MG	1.BR	2. 0. 0.S	300.000 984.000
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.51966419E+01	0.20670254E-01	-0.37253936E-04
0.31937564E-07	-0.99507017E-11	-0.65252617E+05	-0.20288910E+02	
MGBR2(L)	J 6/74MG	1.BR	2. 0. 0.L	984.000 5000.000
0.12580737E+02	0.0	0.0	0.0	0.0
-0.63962980E+05	-0.56255463E+02	0.12580737E+02	0.0	0.0
0.0	0.0	-0.63962980E+05	-0.56255463E+02	
MGBR2	J 6/74MG	1.BR	2. 0. 0.G	300.000 5000.000
0.73215103E+01	0.20643725E-03	-0.92489188E-07	0.18255841E-10	-0.13231169E-14
-0.38671305E+05	-0.56916285E+01	0.57139101E+01	0.77321604E-02	-0.13865793E-04
0.11477901E-07	-0.36057884E-11	-0.38379484E+05	0.18554392E+01	
MGCI	J 3/66MG	1.CL	1.00 0.00 0.G	300.000 5000.000
0.43775835E+01	0.18834179E-03	-0.54488591E-07	0.99481031E-11	-0.66949611E-15
-0.65830820E+04	0.29762335E+01	0.33800535E+01	0.42813383E-02	-0.64457336E-05
0.44472301E-08	-0.11421723E-11	-0.63826562E+04	0.77758331E+01	
MGCI+	J 6/68MG	1.CL	1.E -1.0 0.G	300.000 5000.000
0.63512344E+01	-0.37967190E-02	0.24712945E-05	-0.50823656E-09	0.33672626E-13
0.76480875E+05	-0.83035040E+01	0.36012230E+01	0.34791860E-02	-0.51353145E-05
0.34446337E-08	-0.83848206E-12	0.77314687E+05	0.61207180E+01	

MGCLF J 3/66MG 1.CL 1.F 1.00 0.G 300.000 5000.000
 0.65536108E+01 0.49503800E-03-0.21265566E-06 0.40342910E-10-0.28198241E-14
 -0.70522500E+05-0.61610394E+01 0.39675360E+01 0.10495156E-01-0.14846158E-04
 0.94797308E-08-0.22227489E-11-0.69974500E+05 0.64280834E+01
 MGCI2(S) J12/65MG 1.CI 2.00 0.00 0.S 300.000 987.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.54491301E+01 0.16745225E-01-0.25956906E-04
 0.19111575E-07-0.51059018E-11-0.79343875E+05-0.24261078E+02
 MGCL2(L) J12/65MG 1.CL 2.00 0.00 0.L 987.000 5000.000
 0.11071048E+02 0.0 0.0 0.0 0.0
 -0.76294625E+05-0.48972595E+02 0.11071048E+02 0.0 0.0
 0.0 0.0 -0.76294625E+05-0.48972595E+02
 MGCI2 J12/69MG 1.CL 2.0 0.0 0.G 300.000 5000.000
 0.72401915E+01 0.28856238E-03-0.12401188E-06 0.23527097E-10-0.16443205E-14
 -0.49442324E+05-0.81940546E+01 0.54095526E+01 0.77206269E-02-0.11620094E-04
 0.79417894E-08-0.20252506E-11-0.49070535E+05 0.63400453E+00
 MGF J 3/67MG 1.F 1.00 0.00 0.G 300.000 5000.000
 0.42110739E+01 0.36113267E-03-0.13239531E-06 0.24644425E-10-0.16919093E-14
 -0.28058832E+05 0.23145828E+01 0.28664198E+01 0.51665828E-02-0.65086660E-05
 0.36302039E-08-0.69177563E-12-0.27754852E+05 0.89564753E+01
 MGF2(S) J 3/66MG 1.F 2.00 0.00 0.S 300.000 1536.000
 0.66953754E+01 0.43929182E-02-0.11903585E-05-0.53862115E-09 0.31219775E-12
 -0.13736475E+06-0.32490952E+02 0.21304893E+01 0.28642721E-01-0.45495515E-04
 0.33548645E-07-0.91548253E-11-0.13678475E+06-0.12050724E+02
 MGF2(L) J 3/66MG 1.F 2.00 0.00 0.L 1536.000 5000.000
 0.11357889E+02 0.0 0.0 0.0 0.0
 -0.13400294E+06-0.57018417E+02 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 MGF2 J 3/66MG 1.F 2.00 0.00 0.G 300.000 5000.000
 0.64284668E+01 0.63969987E-03-0.27809762E-06 0.53430246E-10-0.37812838E-14
 -0.89226625E+05-0.60380745E+01 0.37708721E+01 0.10406360E-01-0.13695278E-04
 0.80146521E-08-0.16568864E-11-0.88639625E+05 0.70214052E+01
 MGH J12/66MG 1.H 1.00 0.00 0.G 300.000 5000.000
 0.34638596E+01 0.12404055E-02-0.50278209E-06 0.98118833E-10-0.66183055E-14
 0.19176309E+05 0.29845867E+01 0.35102396E+01-0.12368353E-02 0.64246997E-05
 -0.66054859E-08 0.22003623E-11 0.19293895E+05 0.33604889E+01
 MGN J 3/64MG 1.N 1.00 0.00 0.G 300.000 5000.000
 0.42214413E+01 0.36489242E-03-0.12995730E-06 0.24418939E-10-0.16917759E-14
 0.33382930E+05 0.27188873E+01 0.28894548E+01 0.51757172E-02-0.65849017E-05
 0.37218932E-08-0.72305963E-12 0.33681059E+05 0.92844248E+01
 MGC(S) J12/65MG 1.0 1.00 0.00 0.S 300.000 3098.000
 0.51120195E+01 0.17231663E-02-0.90268816E-06 0.26460611E-09-0.28339967E-13
 -0.74084375E+05-0.26784363E+02 0.47740340E+00 0.21441337E-01-0.33453078E-04
 0.24347436E-07-0.66578965E-11-0.73154250E+05-0.45834875E+01
 MGO(L) J12/65MG 1.0 1.00 0.00 0.L 3098.000 5000.000
 0.72964783E+01 0.0 0.0 0.0 0.0
 -0.67744000E+05-0.38362762E+02 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 MGO J12/65MG 1.0 1.00 0.00 0.G 300.000 5000.000
 0.40654306E+01 0.54784305E-03-0.19704760E-06 0.36606634E-10-0.25102520E-14
 -0.81403809E+03 0.31030931E+01 0.28442078E+01 0.41055530E-02-0.35061248E-05
 0.72885498E-09 0.27783028E-12-0.49777515E+03 0.93349953E+01
 MGOH J 6/67MG 1.0 1.H 1.00 0.G 300.000 5000.000
 0.44328604E+01 0.25811370E-02-0.91887784E-06 0.15151484E-09-0.93758924E-14
 -0.27755887E+05 0.25918925E+00 0.16842604E+01 0.10914847E-01-0.87026992E-05
 0.13936126E-08 0.94723708E-12-0.27081379E+05 0.14150863E+02
 MGOH+ J 6/68MG 1.0 1.H 1.E -1.G 300.000 5000.000
 0.47424326E+01 0.22877008E-02-0.80398934E-06 0.13175298E-09-0.82324454E-14
 0.70323812E+05-0.18812571E+01 0.17246933E+01 0.13231006E-01-0.14929146E-04

0.73413773E-08-0.10182671E-11 0.70977875E+05 0.12933122E+02
 MGO2H2 J 6/67MG 1.0 2.H 2.00 0.G 300.000 5000.000
 0.73269215E+01 0.49370378E-02-0.18021110E-05 0.30460212E-09-0.19535992E-13
 -0.71132812E+05-0.10591697E+02 0.42789288E+01 0.15680924E-01-0.15568570E-04
 0.74423880E-08-0.10867487E-11-0.70438937E+05 0.44899759E+01
 MGS (S) J12/71MG 1.S 1. 0. 0.S 300.000 5000.000
 0.53845549E+01 0.10064589E-02 0.0 0.0 0.0 0.0
 -0.42775512E+05-0.24959839E+02 0.37128267E+01 0.10052007E-01-0.17763858E-04
 0.15086176E-07-0.46961332E-11-0.42537586E+05-0.17430252E+02
 MGS J 6/71MG 1.S 1.0 0.0 0.G 300.000 5000.000
 0.66144295E+01-0.47474876E-02 0.33681108E-05-0.77603701E-09 0.58259495E-13
 0.29105777E+05-0.10003423E+02 0.31967306E+01 0.48075579E-02-0.70028746E-05
 0.46082747E-08-0.10924135E-11 0.30087004E+05 0.77285500E+01
 MGSO4 (S) J 3/66MG 1.S 1.0 4. 0.S 300.000 1400.000
 0.11431275E+02 0.53338408E-02 0.32101807E-05-0.16042432E-08-0.13221412E-12
 -0.15562169E+06-0.56363174E+02 0.36304970E+01 0.38033292E-01-0.46433648E-04
 0.30543315E-07-0.75346110E-11-0.15417906E+06-0.19220093E+02
 MGSO4 (L) J 3/66MG 1.S 1.0 4. 0.L 1400.000 5000.000
 0.19122726E+02 0.0 0.0 0.0 0.0 0.0
 -0.15814794E+06-0.10180466E+03 0.19122726E+02 0.0 0.0
 0.0 0.0 -0.15814794E+06-0.10180466E+03
 MGSI03 (S) J12/67MG 1.SI 1.0 3.0 0.S 300.000 903.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.13377781E+01 0.44453222E-01-0.65973756E-04
 0.47414257E-07-0.12331098E-10-0.18817225E+06-0.10178936E+02
 MGSI03 (S) J12/67MG 1.SI 1.0 3.0 0.S 903.000 1258.000
 0.14473886E+02 0.0 0.0 0.0 0.0 0.0
 -0.19162175E+06-0.76659470E+02 0.14473886E+02 0.0 0.0
 0.0 0.0 -0.19162175E+06-0.76659470E+02
 MGSI03 (S) J12/67MG 1.SI 1.0 3.0 0.S 1258.000 1850.000
 0.14725501E+02 0.0 0.0 0.0 0.0 0.0
 -0.19174200E+06-0.78299301E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 MGSI03 (L) J12/67MG 1.SI 1.0 3.0 0.L 1850.000 5000.000
 0.17613037E+02 0.0 0.0 0.0 0.0 0.0
 -0.18802581E+06-0.95125732E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 MG2SI04 (S) J12/67MG 2.SI 1.0 4.0 0.S 300.000 2171.000
 0.15752679E+02 0.68004653E-02-0.16203949E-05 0.77368112E-11 0.63337573E-13
 -0.26729956E+06-0.81457993E+02 0.13428984E+01 0.66866577E-01-0.96445627E-04
 0.66423979E-07-0.17183990E-10-0.26446900E+06-0.12399162E+02
 MG2SI04 (L) J12/67MG 2.SI 1.0 4.0 0.L 2171.000 5000.000
 0.24658249E+02 0.0 0.0 0.0 0.0 0.0
 -0.26692550E+06-0.13461510E+03 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 MN (S) H11/76MN 1.0 0.0 0.0 0.S 298.150 980.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.27972794E+01 0.10701939E-02 0.19172539E-05
 -0.13918242E-08 0.82299076E-13-0.90643555E+03-0.12508409E+02
 MN H11/76MN 1.0 0.0 0.0 0.G 298.150 2400.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.19650326E+01 0.99111884E-03-0.61388329E-06
 0.13495313E-09-0.43673730E-14 0.33537578E+05 0.96061401E+01
 MO (S) J11/76MO 1.00 0.00 0.00 0.S 298.000 2890.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.24241263E+00 0.43399446E-02-0.91367320E-06
 -0.37895576E-09 0.16121159E-12 0.76171875E+03 0.52051754E+01
 MC (L) J11/76MO 1.00 0.00 0.00 0.L 2890.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0

0.0	0.0	0.11591621E+02	-0.32472757E-02	0.38513508E-06
0.24162325E-10	-0.47644858E-14	-0.95212695E+04	-0.71888504E+02	
MC	J11/76M0	1.00	0.00	0.00
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.51706448E+01	-0.24836680E-02	0.54093505E-06
0.57893024E-10	-0.11490683E-13	0.76443875E+05	-0.88912277E+01	
N	J 3/61N	1.00	0.00	0.00
0.24502678E+01	0.10661458E-03	-0.74653371E-07	0.18796520E-10	-0.10259839E-14
0.56116039E+05	0.44487581E+01	0.25030718E+01	-0.21800181E-04	0.54205287E-07
-0.56475602E-10	0.20999045E-13	0.56098902E+05	0.41675768E+01	
NCO	J12/70N	1.C	1.0	1.0
0.49964361E+01	0.26250880E-02	-0.10928388E-05	0.20309111E-09	-0.13915196E-13
0.17379355E+05	0.17325315E+01	0.31092024E+01	0.66201016E-02	-0.26070084E-05
-0.14966379E-08	0.10922036E-11	0.17977516E+05	0.83561335E+01	
NF	J 6/65N	1.F	1.00	0.00
0.38624048E+01	0.74409950E-03	-0.29304181E-06	0.55130026E-10	-0.38317941E-14
0.28669391E+05	0.34570236E+01	0.30480680E+01	0.19566866E-02	0.94322451E-06
-0.29336642E-08	0.13504458E-11	0.28941687E+05	0.79092360E+01	
NF2	J 3/64N	1.F	2.00	0.00
0.57186890E+01	0.14102822E-02	-0.60493971E-06	0.11491912E-09	-0.80536435E-14
0.30992969E+04	-0.34469261E+01	0.25009871E+01	0.10721061E-01	-0.92064147E-05
0.19027666E-08	0.71249647E-12	0.39376953E+04	0.12994042E+02	
NF3	J 6/69N	1.F	3.0	0.0
0.79819183E+01	0.22349898E-02	-0.96301028E-06	0.18357806E-09	-0.12901443E-13
-0.18673359E+05	-0.15667394E+02	0.12676907E+01	0.24289232E-01	-0.26835973E-04
0.11994192E-07	-0.12905657E-11	-0.17059051E+05	0.17977631E+02	
NH	J12/71N	1.H	1.	0.
0.27789898E+01	0.13266350E-02	-0.41101219E-06	0.69414502E-10	-0.44536179E-14
0.44567973E+05	0.57593431E+01	0.34938316E+01	0.24529034E-03	-0.12578521E-05
0.22011921E-08	-0.92288850E-12	0.44326824E+05	0.18451719E+01	
NH2	J12/65N	1.H	2.00	0.00
0.25769520E+01	0.35896089E-02	-0.12276332E-05	0.19549576E-09	-0.11873400E-13
0.19335910E+05	0.79074888E+01	0.40385790E+01	-0.10098163E-02	0.40120904E-05
-0.23085311E-08	0.39022886E-12	0.18973012E+05	0.52464283E+00	
NH3	J 9/65N	1.H	3.00	0.00
0.24165173E+01	0.61871223E-02	-0.21785136E-05	0.37599079E-09	-0.24448857E-13
-0.64747187E+04	0.77043486E+01	0.35912771E+01	0.49388665E-03	0.83449322E-05
-0.83833385E-08	0.27299092E-11	-0.66717148E+04	0.22520962E+01	
NO	J 6/63N	1.O	1.00	0.00
0.31890001E+01	0.13382281E-02	-0.52899316E-06	0.95919328E-10	-0.64847928E-14
0.98283281E+04	0.67458124E+01	0.40459518E+01	-0.34181783E-02	0.79819192E-05
-0.61139325E-08	0.15919080E-11	0.97453945E+04	0.29974985E+01	
NO+	J 6/66N	1.O	1.E	-1.00
0.28885489E+01	0.15217119E-02	-0.57531241E-06	0.10051081E-09	-0.66044311E-14
0.11819244E+06	0.70027199E+01	0.36685057E+01	-0.11544579E-02	0.21755604E-05
-0.48227466E-09	-0.27847906E-12	0.11803369E+06	0.31779327E+01	
NCCL	J12/72N	1.O	1.CL	1.
0.54178190E+01	0.17391415E-02	-0.67354352E-06	0.12747721E-09	-0.88128391E-14
0.44207891E+04	-0.15287316E+00	0.40453844E+01	0.58322325E-02	-0.54789280E-05
0.27968774E-08	-0.59348674E-12	0.47980586E+04	0.68935318E+01	
NCF	J 6/61N	1.O	1.F	1.00
0.51906662E+01	0.18924265E-02	-0.78642358E-06	0.14626364E-09	-0.10097419E-13
-0.96758164E+04	-0.62298477E+00	0.32902069E+01	0.74045509E-02	-0.66195807E-05
0.26529281E-08	-0.29526815E-12	-0.91566641E+04	0.91451187E+01	
NOP3	J 6/70N	1.O	1.F	3.0
0.98929005E+01	0.33819899E-02	-0.14438137E-05	0.27381675E-09	-0.19186408E-13
-0.23185488E+05	-0.24944305E+02	0.14275875E+01	0.32431848E-01	-0.38573387E-04
0.20510612E-07	-0.37109560E-11	-0.21189426E+05	0.17224289E+02	
NO2	J 9/64N	1.O	2.00	0.00
		0.G	300.000	5000.000

0.46240768E+01	0.25260332E-02	-0.10609501E-05	0.19879239E-09	-0.13799383E-13
0.22899900E+04	0.13324137E+01	0.34589233E+01	0.20647063E-02	0.66866069E-05
-0.95556736E-08	0.36195881E-11	0.28152266E+04	0.83116980E+01	
NC2-	J 6/72N	1.0 2.E 1. 0.G	300.000	5000.000
0.50160904E+01	0.21884462E-02	-0.94586142E-06	0.17939789E-09	-0.12052428E-13
-0.26200160E+05	-0.12861443E+01	0.29818039E+01	0.49398690E-02	0.28557297E-05
-0.78905309E-08	0.35391481E-11	-0.25501539E+05	0.99161682E+01	
NC2CL	J12/65N	1.0 2.CL 1.00 0.G	300.000	5000.000
0.72062140E+01	0.29949809E-02	-0.12641258E-05	0.23758751E-09	-0.16524847E-13
-0.11366123E+04	-0.99256668E+01	0.30302229E+01	0.14538929E-01	-0.11645930E-04
0.25890139E-08	0.64589480E-12	0.76652031E+01	0.11618599E+02	
NC2F	J12/65N	1.0 2.F 1.00 0.G	300.000	5000.000
0.68639164E+01	0.33554437E-02	-0.14158295E-05	0.26622238E-09	-0.18531607E-13
-0.15621285E+05	-0.95806217E+01	0.22424383E+01	0.16289715E-01	-0.13344332E-04
0.32719525E-08	0.59144703E-12	-0.14364203E+05	0.14218996E+02	
NO3	J12/64N	1.0 3. 0. 0.G	300.000	5000.000
0.72033291E+01	0.30908792E-02	-0.13329045E-05	0.25461611E-09	-0.17939047E-13
0.58244023E+04	-0.12608119E+02	0.76867378E+00	0.21181077E-01	-0.16980252E-04
0.22963835E-08	0.19321038E-11	0.75292930E+04	0.20406281E+02	
N2	J 9/65N	2.0 0.0 0.0 0.G	300.000	5000.000
0.28963194E+01	0.15154865E-02	-0.57235275E-06	0.99807398E-10	-0.65223570E-14
-0.90586182E+03	0.61615152E+01	0.36748257E+01	-0.12081501E-02	0.23240100E-05
-0.63217565E-09	-0.22577253E-12	-0.10611587E+04	0.23580427E+01	
N2H4	J12/65N	2.H 4.00 0.00 0.G	300.000	5000.000
0.50947771E+01	0.93296133E-02	-0.33626984E-05	0.56308314E-09	-0.35859662E-13
0.92996641E+04	-0.35950956E+01	0.79803836E+00	0.21788098E-01	-0.13456754E-04
-0.12698753E-09	0.25865213E-11	0.10379887E+05	0.18248703E+02	
N2O	J12/64N	2.0 1.00 0.00 0.G	300.000	5000.000
0.47306681E+01	0.28258266E-02	-0.11558113E-05	0.21263682E-09	-0.14564088E-13
0.81617695E+04	-0.17151070E+01	0.26189194E+01	0.86439624E-02	-0.68110621E-05
0.22275877E-08	-0.80650330E-13	0.87590117E+04	0.92266951E+01	
N2O+	J12/70N	2.0 1.E -1.0 0.G	300.000	5000.000
0.53926945E+01	0.22337197E-02	-0.93548834E-06	0.17466166E-09	-0.12059042E-13
0.15847631E+06	-0.36920185E+01	0.34273062E+01	0.63787699E-02	-0.22585145E-05
-0.20421800E-08	0.13481473E-11	0.15909237E+06	0.67997618E+01	
N2O4	J 9/64N	2.0 4.00 0.00 0.G	300.000	5000.000
0.10506637E+02	0.58723278E-02	-0.24766296E-05	0.46556026E-09	-0.32402083E-13
-0.28609097E+04	-0.26252228E+02	0.36662865E+01	0.23491748E-01	-0.16007296E-04
0.11845940E-08	0.20001622E-11	-0.90631787E+03	0.93973341E+01	
N2O5	J12/64N	2.0 5. 0. 0.G	300.000	5000.000
0.14413736E+02	0.40494092E-02	-0.17661641E-05	0.33912229E-09	-0.23926357E-13
-0.38366062E+04	-0.43313431E+02	0.32144537E+01	0.37992511E-01	-0.36847603E-04
0.12409291E-07	0.24351913E-12	-0.98609497E+03	0.13555831E+02	
N3	J12/70N	3.0 0.0 0.0 0.G	300.000	5000.000
0.51996832E+01	0.24335678E-02	-0.10192343E-05	0.19062350E-09	-0.13212413E-13
0.47963133E+05	-0.35547762E+01	0.30624390E+01	0.73590651E-02	-0.38229373E-05
-0.71824191E-09	0.91110279E-12	0.48614547E+05	0.77570133E+01	
NA(S)	J 6/62NA	1.0 0.0 0.0 O.S	300.000	370.980
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.24118567E+01	0.89751859E-03	0.10583331E-04
-0.71915700E-08	-0.58226618E-11	-0.83578149E+03	-0.82157278E+01	
NA(L)	J 6/62NA	1.0 0.0 0.0 O.L	370.980	2000.000
0.40097370E+01	-0.12933183E-02	0.42443918E-06	0.52381277E-09	-0.18396802E-12
-0.78115479E+03	-0.15366128E+02	0.45673227E+01	-0.25267107E-02	0.14840016E-05
0.38590020E-10	-0.82500846E-13	-0.97421899E+03	0.18377808E+02	
NA	J 6/62NA	1.00 0.00 0.00 0.G	300.000	5000.000
0.25623074E+01	-0.13963284E-03	0.11292707E-06	-0.42307727E-10	0.67057057E-14
0.12193781E+05	0.38957729E+01	0.24881229E+01	0.85426102E-04	-0.21514228E-06
0.22671887E-09	-0.85125266E-13	0.12215902E+05	0.42804842E+01	

NA+ J 3/65NA 1.E -1.00 0.00 0.G 300.000 5000.000
 0.2500000E+01 0.0 0.0 0.0 0.0 0.0
 0.72599312E+05 0.35374012E+01 0.25000000E+01 0.0 0.0 0.0
 0.0 0.0 0.72599312E+05 0.35374012E+01
 NAALSI308(S) GS4/76NA 1.AL 1.SI 3.0 8.S 298.15 1400.00
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.45882416E+02-0.31286784E-01 0.24938403E-04
 0.28272320E-08-0.48666670E-11-0.48498162E+06-0.23009407E+03
 NACL(S) J 9/64NA 1.CL 1.0 0.0 0.S 300.000 1073.800
 0.22134924E+01 0.15859902E-02 0.50486387E-05 0.26020548E-08-0.36487098E-11
 -0.49263203E+05-0.26025658E+01 0.50240774E+01 0.51949061E-02-0.72833727E-05
 0.60671965E-08-0.12013420E-11-0.51123336E+05-0.21227203E+02
 NACL(L) J 9/64NA 1.CL 1.0 0.0 0.L 1073.800 5000.000
 0.12358488E+02-0.63071214E-02 0.32004727E-05-0.67717365E-09 0.51015612E-13
 -0.51423266E+05-0.60585526E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 NACL J 12/64NA 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.44282932E+01 0.15627241E-03-0.28108381E-07 0.47163575E-11-0.28832557E-15
 -0.23170898E+05 0.22878199E+01 0.37032290E+01 0.31997608E-02-0.48924503E-05
 0.34639218E-08-0.91357564E-12-0.23028277E+05 0.57603245E+01
 NAF(S) J 12/68NA 1.F 1.0 0.0 0.S 300.000 1269.000
 0.78342028E+01-0.94839185E-03-0.54843986E-05 0.86843031E-08-0.29285862E-11
 -0.71810375E+05-0.38815704E+02 0.36977549E+01 0.10520574E-01-0.17235652E-04
 0.14125909E-07-0.39514529E-11-0.70647187E+05-0.17393631E+02
 NAF(L) J 12/68NA 1.F 1.0 0.0 0.L 1269.000 3500.000
 0.10963261E+02-0.32068458E-02 0.11611664E-05-0.16299297E-09 0.52456141E-14
 -0.70673937E+05-0.56375702E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 NAF J 12/68NA 1.F 1.0 0.0 0.G 300.000 5000.000
 0.43366880E+01 0.25800569E-03-0.72954947E-07 0.13348457E-10-0.90007563E-15
 -0.36323977E+05 0.12663021E+01 0.31643324E+01 0.49686916E-02-0.72910807E-05
 0.49398423E-08-0.12475984E-11-0.36083203E+05 0.69325352E+01
 NAF2- J 12/68NA 1.F 2.E 1.0 0.G 300.000 5000.000
 0.71223192E+01 0.41884044E-03-0.17972297E-06 0.34041228E-10-0.23751935E-14
 -0.82755750E+05-0.10799851E+02 0.45826893E+01 0.10605212E-01-0.15720507E-04
 0.10567298E-07-0.26415918E-11-0.82234500E+05 0.14760313E+01
 NABC2 J 6/71NA 1.B 1.0 2.0 0.G 300.000 5000.000
 0.74965248E+01 0.26309863E-02-0.10979138E-05 0.20493998E-09-0.14193145E-13
 -0.80578562E+05-0.94594879E+01 0.40654745E+01 0.13454925E-01-0.13866693E-04
 0.66395032E-08-0.10728675E-11-0.79700187E+05 0.79216309E+01
 NABR(S) J 9/64NA 1.BR 1. 0. 0.S 300.000 1020.000
 0.66246452E+01 0.12382983E-03 0.40990278E-06 0.20683651E-09-0.18076486E-13
 -0.45560371E+05-0.27605804E+02 0.48766460E+01 0.68318918E-02-0.10641163E-04
 0.91613934E-08-0.28816298E-11-0.45148645E+05-0.18982544E+02
 NABR(L) J 9/64NA 1.BR 1. 0. 0.L 1020.000 5000.000
 0.74981194E+01 0.0 0.0 0.0 0.0 0.0
 -0.43049770E+05-0.30170456E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 NABR J 9/64NA 1.BR 1. 0. 0.G 300.000 5000.000
 0.44433136E+01 0.15783658E-03-0.27989618E-07 0.53849035E-11-0.38094057E-15
 -0.18659488E+05 0.35954189E+01 0.39010887E+01 0.25025401E-02-0.38851085E-05
 0.28318496E-08-0.77220527E-12-0.18556160E+05 0.61756306E+01
 NACN J 3/66 NA 1.C 1.N 1. 0.G 300.000 5000.000
 0.57989779E+01 0.16827947E-02-0.67437924E-06 0.12234502E-09-0.82966098E-14
 0.94933437E+04-0.43574247E+01 0.49772558E+01 0.53225942E-02-0.75552443E-05
 0.61839778E-08-0.20071427E-11 0.96731484E+04-0.40137136E+00
 NAH J 3/63NA 1.H 1.00 0.00 0.G 300.000 5000.000
 0.38130579E+01 0.85643795E-03-0.31226818E-06 0.58502467E-10-0.40513925E-14
 0.13683062E+05 0.47100288E+00 0.31203947E+01 0.13996216E-02 0.22141230E-05

-0.39950798E-08 0.16726178E-11 0.13940066E+05 0.43813963E+01
 NAI(S) J 9/63NA 1.I 1. 0. 0.S 300.000 933.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.54995985E+01 0.35668053E-02-0.39965626E-05
 0.31841072E-08-0.95308744E-12-0.36390355E+05-0.20399246E+02
 NAI(L) J 9/63NA 1.I 1. 0. 0.L 933.000 5000.000
 0.78000565E+01 0.0 0.0 0.0 0.0 0.0
 -0.34759566E+05-0.30818878E+02 0.78000565E+01 0.0 0.0
 0.0 0.0 -0.34759566E+05-0.30818878E+02
 NAI L 6/72NA 1.I 1. 0. 0.G 300.000 5000.000
 0.44584570E+01 0.14241278E-03-0.16926275E-07 0.38960085E-11-0.27966317E-15
 -0.12066844E+05 0.44627962E+01 0.40406275E+01 0.19687111E-02-0.30545425E-05
 0.22556323E-08-0.62286829E-12-0.11988039E+05 0.64466381E+01
 NAO J12/67NA 1.0 1.0 0.0 0.G 300.000 5000.000
 0.43924160E+01 0.21320574E-03-0.45220599E-07 0.79751821E-11-0.51735989E-15
 0.87118984E+04 0.23749266E+01 0.34421005E+01 0.41617230E-02-0.63118368E-05
 0.44479194E-08-0.11720486E-11 0.89011484E+04 0.69371624E+01
 NAO- J12/67NA 1.0 1.E 1.0 0.G 300.000 5000.000
 0.43868008E+01 0.22344672E-03-0.48212470E-07 0.85720866E-11-0.56094333E-15
 -0.15946270E+05 0.10004511E+01 0.34186859E+01 0.42117387E-02-0.63104644E-05
 0.43873527E-08-0.11372639E-11-0.15752234E+05 0.56553726E+01
 NAOH(S) J12/70NA 1.0 1.H 1.0 0.S 300.000 596.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.85879498E+01-0.35406013E-02-0.45533394E-04
 0.18418484E-06-0.15018974E-09-0.53511852E+05-0.39407578E+02
 NAOH(L) J12/70NA 1.0 1.H 1.0 0.L 596.000 2500.000
 0.94972324E+01 0.22717973E-02-0.23977937E-05 0.78398488E-09-0.81976472E-13
 -0.52906824E+05-0.45299896E+02 0.90556774E+01 0.43025054E-02-0.24259134E-05
 -0.35479664E-08 0.26889420E-11-0.52942445E+05-0.43515137E+02
 NAOH J12/70NA 1.0 1.H 1.0 0.G 300.000 5000.000
 0.56469374E+01 0.12227385E-02-0.33271039E-06 0.40666304E-10-0.17790688E-14
 -0.25508223E+05-0.50500393E+01 0.40050392E+01 0.99922046E-02-0.16434220E-04
 0.12476583E-07-0.34637614E-11-0.25300473E+05 0.22932720E+01
 NAOH+ J12/71NA 1.0 1.H 1.E -1.G 300.000 5000.000
 0.56688547E+01 0.12253930E-02-0.34029563E-06 0.42853263E-10-0.19593761E-14
 0.79806500E+05-0.34378262E+01 0.43505201E+01 0.87465011E-02-0.14642673E-04
 0.11351499E-07-0.32110026E-11 0.79946375E+05 0.23316965E+01
 NA2 J 6/62NA 2.00 0.00 0.00 0.G 300.000 5000.000
 0.44923658E+01 0.19571358E-03 0.22658417E-08-0.10132954E-11 0.10965752E-15
 0.15186082E+05 0.20044165E+01 0.43197517E+01 0.91397949E-03-0.11333877E-05
 0.79289220E-09-0.20379358E-12 0.15220418E+05 0.28326979E+01
 NA2CL2 J12/64NA 2.CL 2.00 0.00 0.G 300.000 5000.000
 0.98262005E+01 0.19184763E-03-0.81608732E-07 0.15298179E-10-0.10558994E-14
 -0.71077125E+05-0.17049255E+02 0.79583950E+01 0.83962344E-02-0.13817116E-04
 0.10277667E-07-0.28644994E-11-0.70725937E+05-0.81884794E+01
 NA2C2N2 J3/66 NA 2.C 2.N 2. 0.G 300.000 5000.000
 0.12572786E+02 0.33947318E-02-0.13616936E-05 0.24720959E-09-0.16773255E-13
 -0.50491016E+04-0.31087357E+02 0.10368029E+02 0.13348546E-01-0.19910338E-04
 0.16156473E-07-0.51264548E-11-0.45937539E+04-0.20562607E+02
 NA2F2 J12/68NA 2.F 2.0 0.0 0.G 300.000 5000.000
 0.94335527E+01 0.63611590E-03-0.27624719E-06 0.52917185E-10-0.37310344E-14
 -0.10480112E+06-0.19766159E+02 0.48212194E+01 0.19836396E-01-0.30617608E-04
 0.21337041E-07-0.55344314E-11-0.10389006E+06 0.23530912E+01
 NA2O(S) J 6/68NA 2.0 1.0 0.0 0.S 300.000 1243.200
 0.24168961E+02-0.25279745E-01-0.47390658E-05 0.31836386E-07-0.14570262E-10
 -0.58048234E+05-0.12518065E+03 0.52654581E+01 0.11116873E-01-0.63875382E-06
 -0.96993205E-08 0.53720075E-11-0.52314344E+05-0.24187027E+02
 NA2O(S) J 6/68NA 2.0 1.0 0.0 0.S 1243.200 1405.200
 -0.14906590E+03 0.22799039E+00 0.38391270E-04-0.17099921E-06 0.61395930E-10

0. 11614797E+05	0.84689258E+03	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
NA2C(L)	J 6/68NA	2.0	1.0	0.0
0.12580737E+02	0.0	0.0	0.0	0.0
-0.48594855E+05	-0.60661545E+02	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
NA20	K10/74NA	2.0	1.	0.
0.71470585E+01	0.39833109E-03	-0.17408911E-06	0.33565165E-10	-0.23810801E-14
-0.72191250E+04	-0.96479731E+01	0.47787180E+01	0.99487714E-02	-0.14814456E-04
0.10003237E-07	-0.25137878E-11	-0.67360195E+04	0.17863131E+01	
NA20H2	J12/70NA	2.0	2.H	2.0
0.94160748E+01	0.55196509E-02	-0.19659610E-05	0.32680347E-09	-0.20712486E-13
-0.76366375E+05	-0.18867508E+02	0.59712934E+01	0.14049277E-01	-0.62445142E-05
-0.33935745E-08	0.28933765E-11	-0.75412937E+05	-0.95055079E+00	
NA2S04(S)	J12/66NA	2.S	1.0	4.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.93771439E+01	0.14655314E-01	0.32944692E-04
-0.52646179E-07	0.12149467E-10	-0.17048000E+06	-0.40806671E+02	
NA2S04(S)	J12/66NA	2.S	1.0	4.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.19418427E+02	0.26281462E-02	-0.87247781E-05
0.20983361E-07	-0.10048205E-10	-0.17199669E+06	-0.92272064E+02	
NA2S04(S)	J12/66NA	2.S	1.0	4.
0.17771698E+02	0.25448797E-02	0.44169556E-05	0.69575634E-09	-0.11463261E-11
-0.17135512E+06	-0.82805862E+02	0.20444046E+02	0.74933560E-04	0.19486879E-05
0.27030962E-08	-0.88779889E-12	-0.17252462E+06	-0.98295456E+02	
NA2S04(L)	J 7/77NA	2.S	1.0	4.
0.23926193E+02	-0.44275820E-03	0.37620794E-06	-0.13448569E-09	0.17195629E-13
0.15460219E+06	-0.11775658E+03	0.18155243E+02	0.15862182E-01	-0.62770210E-04
0.10681600E-06	-0.54320909E-10	0.15739950E+06	-0.84689697E+02	
NA2S04	K11/74NA	2.S	1.0	4.
0.14498731E+02	0.49830154E-02	-0.21511096E-05	0.41120662E-09	-0.28986806E-13
-0.12983756E+06	-0.44400940E+02	0.28682718E+01	0.40050782E-01	-0.37743157E-04
0.11721919E-07	0.81503841E-12	-0.12687350E+06	0.14686440E+02	
NA2SiO3(S)	J 4/76NA	2.SI	1.0	3.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.11987801E+02	0.10751463E-01	-0.23365226E-06
-0.34723382E-08	0.13481265E-11	-0.19202619E+06	-0.58247894E+02	
NA2SiO3(L)	J 4/76NA	2.SI	1.0	3.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.23671539E+02	-0.33039676E-02	0.15625501E-05
-0.25678637E-09	0.40929005E-14	-0.19170806E+06	-0.12208101E+03	
NA2Si205(S)	J 4/76NA	2.SI	2.0	5.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.19980687E+03	-0.48015469E+00	0.25989208E-03
0.22621515E-06	-0.17173769E-09	-0.34719462E+06	-0.10123899E+04	
NA2Si205(L)	J 4/76NA	2.SI	2.0	5.
0.0	0.0	0.0	0.0	0.0
0.0	0.0	0.32023422E+02	-0.14189726E-02	0.11960474E-05
-0.43442272E-09	0.57697228E-13	-0.30541969E+06	-0.16591605E+03	
NE(S)	J12/73NB	1.	0.	0.
0.36736164E+01	-0.15706946E-02	0.19671252E-05	-0.85950935E-09	0.15500611E-12
-0.11241255E+04	-0.16344025E+02	0.25779467E+01	0.19029391E-02	-0.24676383E-05
0.18806743E-08	-0.52837677E-12	-0.83538647E+03	-0.10774210E+02	
NE(L)	J12/73NB	1.	0.	0.
0.40256360E+01	0.0	0.0	0.0	0.0
0.14271587E+04	-0.18580078E+02	0.0	0.0	0.0
0.0	0.0	0.0	0.0	0.0
NB	J12/73NB	1.	0.	0.
0.71470585E+01	0.39833109E-03	-0.17408911E-06	0.33565165E-10	-0.23810801E-14

0.42205906E+01-0.18187440E-02 0.82373941E-06-0.11832899E-09 0.53637040E-14
 0.86960687E+05-0.11978493E+01 0.34755077E+01 0.20538564E-02-0.69670259E-05
 0.68020576E-08-0.22517717E-11 0.87087750E+05 0.22292747E+01
 NBO (S) J12/73NB 1.0 1. 0. 0.S 300.000 2210.000
 0.51236553E+01 0.89375861E-03 0.30930846E-06-0.16433702E-09 0.28569835E-13
 -0.52110910E+05-0.24099518E+02 0.29821262E+01 0.10217544E-01-0.15178895E-04
 0.11308465E-07-0.31382856E-11-0.51703367E+05-0.13918597E+02
 NBO (L) J12/73NB 1.0 1. 0. 0.L 2210.000 5000.000
 0.75484419E+01 0.0 0.0 0.0 0.0
 -0.44587137E+05-0.35817337E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 NBO J12/73NB 1.0 1. 0. 0.G 300.000 5000.000
 0.38811731E+01 0.81978133E-03-0.42535390E-06 0.10264936E-09-0.80419815E-14
 0.22637133E+05 0.62104788E+01 0.29214487E+01 0.31324083E-02-0.14900370E-05
 -0.99345265E-09 0.79984017E-12 0.22907887E+05 0.11223131E+02
 NEO2 (S) J12/73NB 1.0 2. 0. 0.S 300.000 2175.000
 0.17387100E+02-0.84612034E-02-0.23613387E-06 0.29382075E-08-0.80921917E-12
 -0.10262225E+06-0.95054489E+02-0.65260613E+00 0.48355196E-01-0.10658723E-03
 0.11548804E-06-0.45784612E-10-0.96682750E+05-0.35416394E+00
 NBO2 (L) J12/73NB 1.0 2. 0. 0.L 2175.000 5000.000
 0.11322664E+02 0.0 0.0 0.0 0.0
 -0.90623437E+05-0.56772217E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 NB02 J12/73NB 1.0 2. 0. 0.G 300.000 5000.000
 0.59470148E+01 0.11686778E-02-0.50536380E-06 0.96723615E-10-0.68245885E-14
 -0.26058613E+05-0.19232454E+01 0.31937857E+01 0.92979483E-02-0.83422538E-05
 0.21049238E-08 0.44582399E-12-0.25350301E+05 0.12102000E+02
 NB205 (S) J12/72NB 2.0 5. 0. 0.S 300.000 1785.000
 0.17054886E+02 0.49140565E-02 0.47294645E-06-0.18376072E-08 0.50621920E-12
 -0.23423025E+06-0.83224792E+02 0.85053492E+01 0.34401216E-01-0.37698745E-04
 0.19863720E-07-0.39610268E-11-0.23223231E+06-0.40684921E+02
 NE205 (L) J12/72NB 2.0 5. 0. 0.L 1785.000 5000.000
 0.29136993E+02 0.0 0.0 0.0 0.0
 -0.23736025E+06-0.15933395E+03 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 NE L 5/66NE 1.00 0.00 0.00 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0
 -0.74537500E+03 0.33420439E+01 0.250000000E+01 0.0 0.0
 0.0 0.0 -0.74537500E+03 0.33420439E+01
 NE+ L12/66NE 1.E -1.00 0.00 0.G 300.000 5000.000
 0.29285145E+01-0.41229324E-03 0.16341710E-06-0.29554886E-10 0.20056916E-14
 0.25015219E+06 0.24159393E+01 0.21006403E+01 0.32416426E-02-0.56265881E-05
 0.38693067E-08-0.93291347E-12 0.25029537E+06 0.63098679E+01
 NI (S) H10/76NI 1.00 0.00 0.00 0.S 298.15 1726.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.16995945E+01 0.24142351E-02 0.76998276E-06
 -0.11611903E-08 0.24282388E-12-0.29729956E+03-0.61666174E+01
 NI (L) H10/76NI 1.00 0.00 0.00 0.L 1726.00 3200.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.18325378E+02-0.11750482E-01 0.23760622E-05
 0.38630654E-09-0.11958018E-12-0.11077672E+05-0.10877042E+03
 NI H10/76NI 1.00 0.00 0.00 0.G 298.15 3200.00
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.26783218E+01 0.66568144E-03-0.55185518E-06
 0.15237145E-09-0.13882267E-13 0.50958855E+05 0.65245886E+01
 O J 6/740 1. 0. 0. 0.G 300.000 5000.000
 0.25352640E+01-0.14371898E-04-0.11360139E-07 0.66005127E-11-0.61181634E-15
 0.29230266E+05 0.49575624E+01 0.29558659E+01-0.17061536E-02 0.25925156E-05
 -0.17837980E-08 0.45709009E-12 0.29143652E+05 0.29243612E+01

O+ L12/66O 1.E -1.00 0.00 0.G 300.000 5000.000
 0.25060482E+01-0.14464249E-04 0.12446048E-07-0.46858472E-11 0.65548873E-15
 0.18794700E+06 0.43479738E+01 0.24984798E+01 0.11410972E-04-0.29761395E-07
 0.32246539E-10-0.12375517E-13 0.18794906E+06 0.43864355E+01

O- J 6/65O 1.E 1.00 0.00 0.G 300.000 5000.000
 0.25437174E+01-0.53258700E-04 0.25119618E-07-0.51851466E-11 0.39011542E-15
 0.11480516E+05 0.45202541E+01 0.28115797E+01-0.11905697E-02 0.18710552E-05
 -0.13479178E-08 0.36663554E-12 0.11428430E+05 0.32402859E+01

OH J12/700 1.H 1.0 0.0 0.G 300.000 5000.000
 0.29131231E+01 0.95418259E-03-0.19084325E-06 0.12730795E-10 0.24803941E-15
 0.39647061E+04 0.54288731E+01 0.38365517E+01-0.10702014E-02 0.94849759E-06
 0.20843575E-09-0.23384268E-12 0.36715808E+04 0.49805456E+00

OH+ J12/700 1.H 1.E -1.0 0.G 300.000 5000.000
 0.27381496E+01 0.14613173E-02-0.46950538E-06 0.73663561E-10-0.41410933E-14
 0.15761681E+06 0.61343813E+01 0.35365973E+01-0.47029258E-04-0.62344259E-06
 0.17601460E-08-0.82678699E-12 0.15736675E+06 0.18477173E+01

OH- J12/700 1.H 1.E 1.0 0.G 300.000 5000.000
 0.28881149E+01 0.96560223E-03-0.19659257E-06 0.14053802E-10 0.12080617E-15
 -0.18086453E+05 0.41896257E+01 0.34621429E+01 0.40525803E-03-0.13516992E-05
 0.17899460E-08-0.63434810E-12-0.18312355E+05 0.92893219E+00

O2 J 9/65O 2.0 0.0 0.O 300.000 5000.000
 0.36219540E+01 0.73618256E-03-0.19652231E-06 0.36201556E-10-0.28945627E-14
 -0.12019824E+04 0.36150961E+01 0.36255989E+01-0.18782185E-02 0.70554543E-05
 -0.67635142E-08 0.21555995E-11-0.10475227E+04 0.43052778E+01

O2- J12/66O 2.E 1.00 0.00 0.G 300.000 5000.000
 0.38147230E+01 0.77444548E-03-0.30677649E-06 0.56618113E-10-0.38229477E-14
 -0.69910078E+04 0.29587994E+01 0.31440525E+01 0.12127971E-02 0.23812163E-05
 -0.40914081E-08 0.16885304E-11-0.67369766E+04 0.67688684E+01

O3 J 6/61O 3.0 0.0 0.O 300.000 5000.000
 0.54665241E+01 0.17326032E-02-0.72204887E-06 0.13721660E-09-0.96233819E-14
 0.15214098E+05-0.34712620E+01 0.24660616E+01 0.91703199E-02-0.49698483E-05
 -0.20634230E-08 0.20015595E-11 0.16059555E+05 0.12172130E+02

OS(S) H11/760S 1.0 0.0 0.O 298.150 3300.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.33381186E+01-0.28763409E-03 0.39858634E-06
 -0.91004801E-10 0.74708848E-14-0.11274460E+04-0.15281359E+02

OS H11/760S 1.0 0.0 0.O 298.150 5500.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.15040245E+01 0.15054278E-02-0.34504950E-06
 0.42577539E-10-0.21356068E-14 0.94588875E+05 0.14582234E+02

P(S) J 6/61P 1.0 0.0 0.O 300.000 900.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.11869144E+01 0.75957738E-02-0.13635426E-04
 0.13366478E-07-0.47391960E-11-0.59485425E+03-0.57859430E+01

P J 6/62P 1.00 0.00 0.O 300.000 5000.000
 0.26302624E+01-0.17633558E-03 0.12025112E-07 0.39742459E-10-0.56423033E-14
 0.39352992E+05 0.46295137E+01 0.25010147E+01-0.71502000E-05 0.17900987E-07
 -0.19050206E-10 0.73374466E-14 0.39407793E+05 0.53665590E+01

P+ L12/66P 1.E -1.00 0.00 0.G 300.000 5000.000
 0.29021549E+01-0.58878888E-03 0.31298117E-06-0.59727542E-10 0.39304938E-14
 0.16204406E+06 0.38205700E+01 0.43790417E+01-0.64666718E-02 0.89340965E-05
 -0.54858020E-08 0.12098855E-11 0.16174775E+06-0.33068771E+01

PCL3 J 6/70P 1.CI 3.0 0.0 0.G 300.000 5000.000
 0.94566116E+01 0.60278410E-03-0.25846879E-06 0.48904283E-10-0.34083284E-14
 -0.35604613E+05-0.16942810E+02 0.52590532E+01 0.17880566E-01-0.27317583E-04
 0.18898241E-07-0.48738496E-11-0.34764488E+05 0.32391768E+01

PF3 J12/69P 1.F 3.0 0.0 0.G 300.000 5000.000
 0.84347734E+01 0.17393921E-02-0.75119806E-06 0.14344247E-09-0.10093980E-13
 -0.11608081E+06-0.16476761E+02 0.23621874E+01 0.22820044E-01-0.27656642E-04

0.14490961E-07-0.24602360E-11-0.11467694E+06 0.13673269E+02
 PF5 J12/69P 1.F 5.0 0.0 0.G 300.000 5000.000
 0.12846184E+02 0.35104486E-02-0.15198602E-05 0.29101899E-09-0.20534708E-13
 -0.19426231E+06-0.39488708E+02 0.10523252E+01 0.44454005E-01-0.53901429E-04
 0.28416686E-07-0.49143268E-11-0.19153237E+06 0.19075851E+02
 PH J 6/67P 1.H 1.00 0.00 0.G 300.000 5000.000
 0.30745440E+01 0.11698946E-02-0.30381653E-06 0.44436316E-10-0.27000975E-14
 0.29526773E+05 0.57548838E+01 0.36803436E+01-0.12756018E-02 0.25932441E-05
 -0.84354101E-09-0.17208609E-12 0.29433910E+05 0.29054766E+01
 PH3 J 6/62P 1.H 3.00 0.00 0.G 300.000 5000.000
 0.33448792E+01 0.65770932E-02-0.26336756E-05 0.47744653E-09-0.32354389E-13
 0.12837666E+04 0.39416275E+01 0.31581936E+01 0.24941491E-02 0.90255253E-05
 -0.10227904E-07 0.32834247E-11 0.16387061E+04 0.62240562E+01
 PN J 9/62P 1.N 1.00 0.00 0.G 300.000 5000.000
 0.36419230E+01 0.94460673E-03-0.38923480E-06 0.73215822E-10-0.50961636E-14
 0.11393687E+05 0.41772776E+01 0.33755236E+01-0.41009393E-03 0.51265151E-05
 -0.59478893E-08 0.21213578E-11 0.11578840E+05 0.60897417E+01
 PO J 6/71P 1.O 1. 0. 0.G 300.000 5000.000
 0.38427925E+01 0.72364463E-03-0.28934198E-06 0.53013552E-10-0.35495373E-14
 -0.26995117E+04 0.45392141E+01 0.39613075E+01-0.21235398E-02 0.75201215E-05
 -0.75950908E-08 0.25637591E-11-0.25990256E+04 0.45705290E+01
 PS J 6/67P 1.S 1.00 0.00 0.G 300.000 5000.000
 0.43563528E+01 0.20240866E-03-0.78680671E-07 0.15193430E-10-0.81648513E-15
 0.93838320E+04 0.32161160E+01 0.37492027E+01 0.24330574E-02-0.31107902E-05
 0.17650761E-08-0.34208790E-12 0.95171445E+04 0.61975908E+01
 P2 J 6/61P 2.00 0.00 0.00 0.G 300.000 5000.000
 0.41611729E+01 0.39620791E-03-0.15580338E-06 0.29093478E-10-0.20042458E-14
 0.20146758E+05 0.22279291E+01 0.28391104E+01 0.48266202E-02-0.54947486E-05
 0.25800506E-08-0.32236453E-12 0.20459594E+05 0.88292475E+01
 P4 J 6/61P 4.00 0.00 0.00 0.G 300.000 5000.000
 0.92262793E+01 0.86894119E-03-0.37758338E-06 0.72379672E-10-0.51066126E-14
 0.12490324E+05-0.19654861E+02 0.35353298E+01 0.24125293E-01-0.36462763E-04
 0.24916908E-07-0.63298559E-11 0.13635309E+05 0.77427330E+01
 P4010(S) GS3/77P 4.0 10. 0. 0.S 400.00 900.00
 0.0 0.0 0. 0. 0. 0.0
 0.0 0.0 0.14087844E+02 0.39084297E-01 0.32008305E-04
 -0.22006894E-07 0.20300090E-11-0.33340925E+06-0.66045090E+02
 PB(S) J 3/62PB 1. 0. 0. 0.S 300.000 600.580
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.29429770E+01 0.40499610E-03 0.37401314E-05
 -0.81217273E-08 0.58517505E-11-0.91582983E+03-0.92034760E+01
 PB(L) J 3/62PB 1. 0. 0. 0.L 600.580 3000.000
 0.49864931E+01-0.27910068E-02 0.17157026E-05-0.41012216E-09 0.34690190E-13
 -0.10290974E+04-0.19437302E+02 0.37698584E+01 0.73868345E-04-0.33181522E-06
 -0.15598935E-09 0.17983515E-12-0.65495630E+03-0.12995204E+02
 PB J 3/62PB 1. 0. 0. 0.G 300.000 5000.000
 0.42593222E+01-0.36850709E-02 0.24028450E-05-0.50662297E-09 0.34722632E-13
 0.22181523E+05-0.26731281E+01 0.25026388E+01-0.28137962E-04 0.10347173E-06
 -0.15731530E-09 0.84539309E-13 0.22778910E+05 0.68254757E+01
 PBBR J12/73PB 1.BR 1. 0. 0.G 300.000 5000.000
 0.47268763E+01-0.43918379E-03 0.33215582E-06-0.65307246E-10 0.42726104E-14
 0.70988945E+04 0.58541889E+01 0.41906843E+01 0.13411178E-02-0.20978996E-05
 0.15510908E-08-0.42617911E-12 0.72369453E+04 0.85616150E+01
 PBBR2(S) J12/73PB 1.BR 2. 0. 0.S 300.000 644.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.10557554E+02-0.70617385E-02 0.10187602E-04
 0.13052876E-07-0.16373097E-10-0.36304801E+05-0.39199036E+02
 PBBR2(L) J12/73PB 1.BR 2. 0. 0.L 644.000 5000.000
 0.13486549E+02 0.0 0.0 0.0 0.0

-0.36572199E+05-0.57049088E+02 0.13486549E+02 0.0 0.0
 0.0 0.0 -0.36572199E+05-0.57049088E+02
 PBBR2 J12/73PB 1.BR 2. 0. 0.G 300.000 5000.000
 0.69472904E+01 0.60199003E-04-0.26556684E-07 0.51596010E-11-0.36837061E-15
 -0.14645441E+05 0.11669950E+01 0.63902092E+01 0.25289049E-02-0.41903741E-05
 0.31367522E-08-0.87976745E-12-0.14541793E+05 0.38043661E+01
 PBBR4 J12/73PB 1.BR 4. 0. 0.G 300.000 5000.000
 0.12856973E+02 0.16323940E-03-0.71970362E-07 0.13975749E-10-0.99736181E-15
 -0.58772094E+05-0.22158920E+02 0.11379366E+02 0.66625886E-02-0.10940648E-04
 0.81094740E-08-0.22495573E-11-0.58495430E+05-0.15153331E+02
 PBCL J 6/73PB 1.CL 1. 0. 0.G 300.000 5000.000
 0.47016535E+01-0.42255176E-03 0.32684778E-06-0.65162153E-10 0.42978587E-14
 0.37797998E+03 0.44242802E+01 0.38972912E+01 0.24867463E-02-0.39157148E-05
 0.28494282E-08-0.77266579E-12 0.56862573E+03 0.84153128E+01
 PBCL+ J 6/73PB 1.CL 1.E -1. 0.G 300.000 5000.000
 0.44591694E+01 0.97407305E-04-0.48821143E-08-0.25472246E-11 0.62470882E-15
 0.88325875E+05 0.51999426E+01 0.39604807E+01 0.22511384E-02-0.35559306E-05
 0.26130964E-08-0.71901285E-12 0.88421375E+05 0.75745850E+01
 PBCL2 (S) J 6/73PB 1.CL 2. 0. 0.S 300.000 774.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.82802687E+01 0.30414343E-02 0.15602582E-05
 -0.22284610E-08 0.11115440E-11-0.45841219E+05-0.31781235E+02
 PBCL2 (L) J 6/73PB 1.CL 2. 0. 0.L 774.000 5000.000
 0.13411065E+02 0.0 0.0 0.0 0.0
 -0.46167078E+05-0.59932648E+02 0.13411065E+02 0.0 0.0
 0.0 0.0 -0.46167078E+05-0.59932648E+02
 PBCL2 J 6/73PB 1.CL 2. 0. 0.G 300.000 5000.000
 0.68401680E+01 0.20601308E-03-0.10023433E-06 0.19262772E-10-0.87941417E-15
 -0.23016363E+05-0.97691488E+00 0.56399403E+01 0.54622144E-02-0.88056868E-05
 0.64197216E-08-0.17518591E-11-0.22792336E+05 0.47147455E+01
 PBCL2+ J 6/73PB 1.CL 2.E -1. 0.G 300.000 5000.000
 0.68418837E+01 0.19792473E-03-0.96562815E-07 0.20106444E-10-0.13246579E-14
 0.96094000E+05-0.82920027E+00 0.55653877E+01 0.57468414E-02-0.92445043E-05
 0.67256885E-08-0.18313857E-11 0.96335000E+05 0.52358971E+01
 PBCL4 J12/73PB 1.CL 4. 0. 0.G 300.000 5000.000
 0.12669673E+02 0.37512253E-03-0.16465373E-06 0.31848857E-10-0.22650946E-14
 -0.70329125E+05-0.26636993E+02 0.96282978E+01 0.13456438E-01-0.21571730E-04
 0.15638214E-07-0.42414926E-11-0.69746500E+05-0.12148006E+02
 PBF J12/73PB 1.F 1. 0. 0.G 300.000 5000.000
 0.46052198E+01-0.32622227E-03 0.28298251E-06-0.57120600E-10 0.37397826E-14
 -0.11086918E+05 0.37274313E+01 0.32454481E+01 0.46936162E-02-0.69780026E-05
 0.47459316E-08-0.11983929E-11-0.10777074E+05 0.10430569E+02
 PBF2 (S) J12/73PB 1.F 2. 0. 0.S 300.000 583.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.13320626E+02-0.57548907E-01 0.24546310E-03
 -0.44016599E-06 0.29332003E-09-0.84387187E+05-0.52915543E+02
 PBF2 (S) J12/73PB 1.F 2. 0. 0.S 583.000 1103.000
 -0.18691818E+02 0.21901701E-01 0.26912981E-04-0.32722531E-08-0.15183577E-10
 -0.70641437E+05 0.12567334E+03-0.28540552E+03 0.79433262E+00-0.99227269E-04
 -0.10663989E-05 0.66836603E-09-0.19024777E+05 0.14421931E+04
 PBF2 (L) J12/73PB 1.F 2. 0. 0.L 1103.000 5000.000
 0.13134289E+02 0.0 0.0 0.0 0.0
 -0.84759750E+05-0.62193268E+02 0.0 0.0 0.0
 0.0 0.0 0.0
 PBF2 J12/73PB 1.F 2. 0. 0.G 300.000 5000.000
 0.66354589E+01 0.41173119E-03-0.18004607E-06 0.34728984E-10-0.24645269E-14
 -0.54425059E+05-0.29600248E+01 0.41295691E+01 0.10561626E-01-0.15808138E-04
 0.10725749E-07-0.27093891E-11-0.53916121E+05 0.91272621E+01
 PBF4 J12/73PB 1.F 4. 0. 0.G 300.000 5000.000

0.12127774E+02 0.98421052E-03-0.43006162E-06 0.82902421E-10-0.58800214E-14
 -0.14020344E+06-0.29804108E+02 0.62745390E+01 0.24576280E-01-0.36567537E-04
 0.24663265E-07-0.61876008E-11-0.13900919E+06-0.15427485E+01
 PBI J12/73PB 1.I 1. 0. 0.G 300.000 5000.000
 0.47186108E+01-0.41882228E-03 0.30970847E-06-0.59203351E-10 0.38773983E-14
 0.11534109E+05 0.68260307E+01 0.43073397E+01 0.85668243E-03-0.13164554E-05
 0.97187236E-09-0.26526746E-12 0.11645742E+05 0.89281664E+01
 PBI2(S) J12/73PB 1.I 2. 0. 0.S 300.000 683.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.84424429E+01 0.59195757E-02-0.13888686E-04
 0.13221392E-07 0.16164067E-11-0.23779051E+05-0.28337906E+02
 PBI2(L) J12/73PB 1.I 2. 0. 0.L 683.000 5000.000
 C.13058805E+02 0.0 0.0 0.0 0.0 0.0
 -0.23440934E+05-0.52044800E+02 0.13058805E+02 0.0 0.0
 0.0 0.0 -0.23440934E+05-0.52044800E+02
 PBI2 J12/73PB 1.I 2. 0. 0.G 300.000 5000.000
 0.69761105E+01 0.27474569E-04-0.12204215E-07 0.23862492E-11-0.17133768E-15
 -0.24707898E+04 0.34585733E+01 0.67169228E+01 0.11849878E-02-0.19791551E-05
 0.14927377E-08-0.42189646E-12-0.24229504E+04 0.46835928E+01
 PBI4 J12/73PB 1.I 4. 0. 0.G 300.000 5000.000
 0.12927661E+02 0.82998289E-04-0.36781667E-07 0.71764296E-11-0.51430951E-15
 -0.30877629E+05-0.17668915E+02 0.12150266E+02 0.35387082E-02-0.58782434E-05
 0.44072159E-08-0.12374051E-11-0.30733566E+05-0.13991295E+02
 PBS(S) J 6/73PB 1.S 1. 0. 0.S 300.000 1386.500
 0.48695412E+01 0.25509847E-02-0.38042879E-06-0.54814642E-09 0.26573817E-12
 -0.13298453E+05-0.17299606E+02 0.55160971E+01 0.17196687E-02-0.12658602E-05
 0.12505685E-08-0.46278508E-12-0.13538180E+05-0.20909271E+02
 PBS(L) J 6/73PB 1.S 1. 0. 0.L 1386.500 5000.000
 0.80516710E+01 0.0 0.0 0.0 0.0 0.0
 -0.13566059E+05-0.35757797E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 PBS J 6/73PB 1.S 1. 0. 0.G 300.000 5000.000
 0.40911522E+01 0.83885365E-03-0.57157206E-06 0.16160476E-09-0.12511896E-13
 0.14601695E+05 0.66875477E+01 0.34774532E+01 0.39700307E-02-0.61096689E-05
 0.43008690E-08-0.11311551E-11 0.14684750E+05 0.94646091E+01
 PB2 J 9/63PB 2. 0. 0. 0.G 300.000 5000.000
 0.44598341E+01 0.24006380E-03-0.19259861E-07 0.36456940E-11-0.25380940E-15
 0.38654051E+05 0.83117971E+01 0.40501223E+01 0.20230000E-02-0.29701350E-05
 0.21785957E-08-0.59755326E-12 0.38731641E+05 0.10258829E+02
 PD(S) H11/76PD 1.0 0.0 0.0 0.S 298.150 1825.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.26632977E+01 0.12133375E-02-0.10272112E-06
 -0.33700176E-09 0.16117641E-12-0.81803052E+03-0.10912824E+02
 PD H11/76PD 1.0 0.0 0.0 0.G 298.150 3300.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.54267683E+01 0.72183423E-02-0.84949033E-06
 -0.22023010E-09 0.32322255E-13 0.49686883E+05 0.54280640E+02
 PI(S) H11/76PT 1.0 0.0 0.0 0.S 298.150 2042.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.34152308E+01-0.41113514E-03 0.77377348E-06
 -0.21709111E-09 0.15300695E-13-0.10733286E+04-0.14503420E+02
 PI H11/76PT 1.0 0.0 0.0 0.G 298.150 4000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.17761097E+01 0.10684791E-02-0.49331163E-06
 0.10989279E-09-0.88535373E-14 0.68036625E+05 0.13864265E+02
 RE(S) H11/76RE 1.0 0.0 0.0 0.S 298.150 3453.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.32329664E+01 0.76051656E-04 0.31713591E-06
 -0.74897158E-10 0.64558649E-14-0.10753071E+04-0.14089895E+02

RE H11/76RE 1.0 0.0 0.0 0.G 298.150 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.30531206E+01-0.13315075E-02 0.45616798E-06
 0.26633779E-10-0.82542581E-14 0.92870687E+05 0.60343742E+01
 RH(S) H11/76RH 1.0 0.0 0.0 0.S 298.150 2233.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.28894415E+01 0.72652637E-03 0.46660045E-06
 -0.25907609E-09 0.32073292E-13-0.94131543E+03-0.12994571E+02
 RH H11/76RH 1.0 0.0 0.0 0.G 298.150 4000.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.28747702E+01 0.61959727E-03-0.30569385E-06
 0.63584513E-10-0.43965177E-14 0.65448832E+05 0.53796539E+01
 RU(S) H11/76RU 1.0 0.0 0.0 0.S 298.150 2523.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.33040695E+01-0.68073231E-03 0.79932136E-06
 -0.43282988E-10-0.20714895E-13-0.10257397E+04-0.15381838E+02
 RU H11/76RU 1.0 0.0 0.0 0.G 298.150 4500.000
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.12754078E+01 0.14420375E-02-0.29576768E-06
 0.33752806E-10-0.18905214E-14 0.78867687E+05 0.16078262E+02
 S(S) J12/65S 1.0 0.0 0.0 0.S 300.000 388.360
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.50637026E+01 0.28819353E-02-0.21330212E-04
 0.84787860E-06-0.17344968E-08 0.71482617E+03 0.28714081E+02
 S(L) J12/65S 1.0 0.0 0.0 0.L 388.360 2000.000
 0.36036673E+01 0.99033397E-03-0.10114409E-05 0.40536330E-09-0.56679135E-13
 -0.84538379E+03-0.16344711E+02-0.12706310E+02 0.90725243E-01-0.16951787E-03
 0.13070638E-06-0.35276143E-10 0.12346069E+04 0.56210159E+02
 S J 6/71S 1.0 0.0 0.0 0.G 300.000 5000.000
 0.29093332E+01-0.55587292E-03 0.27836950E-06-0.50194765E-10 0.31254639E-14
 0.32531543E+05 0.37928324E+01 0.29270077E+01 0.21982555E-03-0.23808852E-05
 0.29034821E-08-0.10846688E-11 0.32491578E+05 0.35120602E+01
 S+ L12/66S 1.E -1.00 0.00 0.G 300.000 5000.000
 0.24118652E+01 0.22103303E-03-0.18939562E-06 0.61886676E-10-0.53887728E-14
 0.15375731E+06 0.58861132E+01 0.25088215E+01-0.62478561E-04 0.15513302E-06
 -0.16148749E-09 0.60012108E-13 0.15373000E+06 0.53857183E+01
 SF4 J12/69S 1.F 4.0 0.0 0.G 300.000 5000.000
 0.11101043E+02 0.21130999E-02-0.91283096E-06 0.17427082E-09-0.12258515E-13
 -0.97712750E+05-0.28685410E+02 0.24622421E+01 0.33574536E-01-0.43722175E-04
 0.25301102E-07-0.51523829E-11-0.95788562E+05 0.13841967E+02
 SF6 J 9/65S 1.F 6.00 0.00 0.G 300.000 5000.000
 0.15286816E+02 0.41541271E-02-0.18053252E-05 0.34670689E-09-0.24523633E-13
 -0.15234675E+06-0.55069672E+02-0.11646700E+01 0.64060926E-01-0.83337509E-04
 0.48244601E-07-0.98455246E-11-0.14868150E+06 0.25921768E+02
 SH J 6/67S 1.H 1.00 0.00 0.G 300.000 5000.000
 0.30371380E+01 0.12752465E-02-0.42314343E-06 0.67719663E-10-0.40934324E-14
 0.16545437E+05 0.60722980E+01 0.44098949E+01-0.22063747E-02 0.13171084E-05
 0.16467179E-08-0.12144790E-11 0.16180734E+05-0.10226126E+01
 SN J 6/61S 1.N 1.00 0.00 0.G 300.000 5000.000
 0.38493977E+01 0.72756782E-03-0.29370204E-06 0.55013633E-10-0.38123564E-14
 0.30459961E+05 0.44179134E+01 0.39422970E+01-0.20035515E-02 0.73534648E-05
 -0.75168565E-08 0.25591100E-11 0.30563949E+05 0.45669479E+01
 SO J 6/71S 1.0 1.0 0.0 0.G 300.000 5000.000
 0.40039062E+01 0.29471354E-03 0.63481139E-07-0.28687400E-10 0.25022781E-14
 -0.72238721E+03 0.35413675E+01 0.31258707E+01 0.13512855E-02 0.21503884E-05
 -0.39964441E-08 0.17048142E-11-0.41679712E+03 0.84036007E+01
 SOF2 J 6/72S 1.0 1.F 2. 0.G 300.000 5000.000
 0.80874214E+01 0.21095716E-02-0.90866911E-06 0.17344834E-09-0.12214158E-13
 -0.68238187E+05-0.13868859E+02 0.24749069E+01 0.20952426E-01-0.24164270E-04

0.12120378E-07-0.19338732E-11-0.66897625E+05 0.14184073E+02
 SC2 J 6/61S 1.0 2.00 0.00 0.G 300.000 5000.000
 0.52451363E+01 0.19704204E-02-0.80375770E-06 0.15149969E-09-0.10558005E-13
 -0.37558227E+05-0.10873528E+01 0.32665339E+01 0.53237900E-02 0.68437549E-06
 -0.52810059E-08 0.25590450E-11-0.36908148E+05 0.96513472E+01
 SO2CL2 J 6/71S 1.0 2.CL 2.0 0.G 300.000 5000.000
 0.10550937E+02 0.26734301E-02-0.11428228E-05 0.21686200E-09-0.15199152E-13
 -0.46295055E+05-0.24321075E+02 0.43851681E+01 0.23212157E-01-0.26532114E-04
 0.13499925E-07-0.22819281E-11-0.44802973E+05 0.65654554E+01
 SC2CLF J 6/71S 1.0 2.CL 1.F 1.G 300.000 5000.000
 0.10118286E+02 0.31488994E-02-0.13471517E-05 0.25580316E-09-0.17938257E-13
 -0.70509312E+05-0.23141083E+02 0.29817524E+01 0.26449166E-01-0.29200179E-04
 0.13957610E-07-0.20304487E-11-0.68761500E+05 0.12718446E+02
 SO2F2 J 6/71S 1.0 2.F 2.0 0.G 300.000 5000.000
 0.96078882E+01 0.37111025E-02-0.15899113E-05 0.30232461E-09-0.21228577E-13
 -0.94754750E+05-0.22862198E+02 0.17324677E+01 0.28501760E-01-0.29453804E-04
 0.12401301E-07-0.11715533E-11-0.92781375E+05 0.16935165E+02
 S03 J 9/65S 1.0 3.00 0.00 0.G 300.000 5000.000
 0.70757380E+01 0.31763387E-02-0.13535764E-05 0.25630920E-09-0.17936045E-13
 -0.50211375E+05-0.11200793E+02 0.25780382E+01 0.14556333E-01-0.91764177E-05
 -0.79203022E-09 0.19709477E-11-0.48931754E+05 0.12251863E+02
 S2 J12/65S 2.00 0.00 0.00 0.G 300.000 5000.000
 0.42051134E+01 0.35309140E-03-0.13543070E-06 0.25245375E-10-0.17357488E-14
 0.14182906E+05 0.32094717E+01 0.28724251E+01 0.50434470E-02-0.62055278E-05
 0.53097023E-08-0.57376109E-12 0.14487074E+05 0.98082409E+01
 S8 J6/64 S 8. 0. 0. 0.G 300.000 5000.000
 0.20751770E+02 0.14126296E-02-0.61834766E-06 0.11933438E-09-0.84707665E-14
 0.55882539E+04-0.67731583E+02 0.10602257E+02 0.44008818E-01-0.68651731E-04
 0.48505850E-07-0.12808281E-10 0.75807969E+04-0.19129654E+02
 SI(S) J 3/67SI 1.00 0.00 0.00 0.S 300.000 1685.000
 0.24753990E+01 0.88112196E-03-0.20939478E-06 0.42757187E-11 0.16006565E-13
 -0.81255615E+03-0.12188747E+02 0.84197539E+00 0.83710402E-02-0.13077030E-04
 0.97593613E-08-0.27279377E-11-0.52486279E+03-0.45272675E+01
 SI(L) J 3/67SI 1.00 0.00 0.00 0.I 1685.000 5000.000
 0.32709913E+01 0.0 0.0 0.0 0.0 0.0 0.0
 0.48546562E+04-0.13289281E+02 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0 0.0
 SI J 3/67SI 1.00 0.00 0.00 0.G 300.000 5000.000
 0.26506014E+01-0.35763858E-03 0.29592292E-06-0.72804832E-10 0.57963345E-14
 0.53437055E+05 0.52204056E+01 0.31793537E+01-0.27646993E-02 0.44784038E-05
 -0.32833176E-08 0.91213669E-12 0.53339031E+05 0.27273207E+01
 SI+ J12/71SI 1.E -1. 0. 0.G 300.000 5000.000
 0.26571112E+01-0.18079509E-03 0.80092263E-07-0.15634896E-10 0.11244002E-14
 0.14877200E+06 0.46696587E+01 0.39715433E+01-0.55429116E-02 0.83573022E-05
 -0.56676122E-08 0.14235783E-11 0.14850806E+06-0.16582212E+01
 SIC J 3/67SI 1.C 1.00 0.00 0.G 300.000 5000.000
 0.55799036E+01-0.13409343E-02 0.75483047E-06-0.16543777E-09 0.12663346E-13
 0.85046125E+05-0.56633596E+01-0.21924696E+01 0.41342702E-01-0.78274112E-04
 0.60694106E-07-0.16729201E-10 0.85953125E+05 0.28756073E+02
 SIC2 J 3/67SI 1.C 2.00 0.00 0.G 300.000 5000.000
 0.57011518E+01 0.21220690E-02-0.11457769E-05 0.31038772E-09-0.27763897E-13
 0.72023375E+05-0.49868956E+01 0.38806334E+01 0.67947768E-02-0.50277959E-05
 0.10573231E-08 0.25513142E-12 0.72558250E+05 0.45374041E+01
 SICL J 9/67SI 1.CL 1.00 0.00 0.G 300.000 5000.000
 0.44179420E+01 0.13137081E-03-0.30789014E-07 0.47802942E-11-0.24135145E-15
 0.21650363E+05 0.33226347E+01 0.38247528E+01 0.24969131E-02-0.36640267E-05
 0.25169051E-08-0.65148061E-12 0.21774074E+05 0.61967573E+01
 SICL2 J12/70SI 1.CL 2.0 0.0 0.G 300.000 5000.000
 0.66562014E+01 0.39225514E-03-0.16975918E-06 0.30024025E-10-0.14765027E-14

-0.22217441E+05-0.43502102E+01 0.42340631E+01 0.10291979E-01-0.15513724E-04
 0.10572098E-07-0.26771632E-11-0.21730887E+05 0.73084888E+01
 SICL3 J12/69SI 1.CI 3.0 0.0 0.G 300.000 5000.000
 0.93913631E+01 0.67983521E-03-0.29385990E-06 0.56056340E-10-0.39374869E-14
 -0.51298469E+05-0.15758539E+02 0.51253424E+01 0.17938811E-01-0.26825408E-04
 0.18160893E-07-0.45701854E-11-0.50431047E+05 0.48235054E+01
 SICL4 J12/70SI 1.CL 4.0 0.0 0.G 300.000 5000.000
 0.12089655E+02 0.10190734E-02-0.44167865E-06 0.84481575E-10-0.59491596E-14
 -0.83590250E+05-0.29940079E+02 0.61040010E+01 0.24933115E-01-0.36703263E-04
 0.24448749E-07-0.60370155E-11-0.82359250E+05-0.98955292E+00
 SIF J12/69SI 1.F 1.0 0.0 0.G 300.000 5000.000
 0.41433077E+01 0.42824983E-03-0.16212960E-06 0.29310637E-10-0.18339280E-14
 -0.36327053E+04 0.32628908E+01 0.33086576E+01 0.25106061E-02-0.13181489E-05
 -0.67703843E-09 0.61282750E-12-0.34002393E+04 0.76058826E+01
 SIF2 J12/68SI 1.F 2.0 0.0 0.G 300.000 5000.000
 0.60359097E+01 0.11232006E-02-0.51341254E-06 0.10234931E-09-0.69009299E-14
 -0.72721125E+05-0.42661200E+01 0.29365749E+01 0.11439476E-01-0.12803853E-04
 0.58541332E-08-0.68518585E-12-0.71985437E+05 0.11224577E+02
 SIF3 J 6/70SI 1.F 3.0 0.0 0.G 300.000 5000.000
 0.84105120E+01 0.17564832E-02-0.75509757E-06 0.14362943E-09-0.10073780E-13
 -0.13523387E+06-0.15189859E+02 0.30581579E+01 0.19504987E-01-0.21991975E-04
 0.10298763E-07-0.13244718E-11-0.13395275E+06 0.11596386E+02
 SIF4 J 9/63SI 1.F 4.00 0.00 0.G 300.000 5000.000
 0.10545038E+02 0.27200801E-02-0.11741276E-05 0.22433362E-09-0.15803155E-13
 -0.19792287E+06-0.27951950E+02 0.31059752E+01 0.26866991E-01-0.29186296E-04
 0.12874580E-07-0.13617267E-11-0.19611325E+06 0.94141922E+01
 SIH J12/69SI 1.H 1.0 0.0 0.G 300.000 5000.000
 0.30911188E+01 0.14689346E-02-0.56349950E-06 0.10071335E-09-0.63679395E-14
 0.44302445E+05 0.57808352E+01 0.41309786E+01-0.35619084E-02 0.76432634E-05
 -0.53797073E-08 0.12582730E-11 0.44159598E+05 0.10358458E+01
 SIH+ J12/71SI 1.H 1.E -1. 0.G 300.000 5000.000
 0.29828596E+01 0.15455221E-02-0.59038553E-06 0.10517399E-09-0.68220237E-14
 0.13707956E+06 0.50272131E+01 0.37292585E+01-0.17881610E-02 0.42469255E-05
 -0.25580129E-08 0.40633740E-12 0.13697069E+06 0.15707359E+01
 SIH4 J12/60SI 1.H 4.00 0.00 0.G 300.000 5000.000
 0.44433851E+01 0.86334199E-02-0.35060002E-05 0.64194983E-09-0.43824526E-13
 0.18468284E+04-0.40777750E+01 0.17519579E+01 0.11664484E-01 0.10686372E-05
 -0.75C58679E-08 0.31897219E-11 0.28880916E+04 0.11103122E+02
 SIN J 3/67SI 1.N 1.00 0.00 0.G 300.000 5000.000
 0.39858618E+01-0.87927056E-05 0.54269537E-06-0.17951017E-09 0.16337070E-13
 0.43524809E+05 0.31615152E+01 0.31051950E+01 0.14852448E-02 0.18561059E-05
 -0.37734900E-08 0.16835335E-11 0.43785711E+05 0.78753958E+01
 SIO J 9/67SI 1.0 1.00 0.00 0.G 300.000 5000.000
 0.37478838E+01 0.81991940E-03-0.32525395E-06 0.57324964E-10-0.35108944E-14
 -0.13317430E+05 0.36478405E+01 0.32528276E+01 0.41823136E-03 0.37806203E-05
 -0.51024500E-08 0.19471317E-11-0.13090340E+05 0.66485806E+01
 SIO2(S) J 6/67SI 1.0 2.00 0.00 0.S 300.000 847.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.37282163E+00 0.21562222E-01-0.14573894E-04
 -0.89309893E-08 0.12526015E-10-0.11048162E+06-0.28621540E+01
 SIO2(S) J 6/67SI 1.0 2.00 0.00 0.S 847.000 1079.000
 0.70854712E+01 0.12077508E-02 0.0 0.0 0.0 0.0
 -0.11178737E+06-0.36198181E+02 0.70854712E+01 0.12077508E-02 0.0
 0.0 0.0 -0.11178737E+06-0.36198181E+02
 SIO2(S) J 6/67SI 1.0 2.00 0.00 0.S 1079.000 1996.000
 0.66032381E+01 0.25956500E-02-0.69075293E-06-0.17559104E-09 0.82131513E-13
 -0.11150869E+06-0.33656250E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0 0.0
 SIO2(L) J 6/67SI 1.0 2.00 0.00 0.L 300.000 4500.000

0.56108065E+01 0.32523847E-02-0.22449939E-06-0.21156407E-09 0.34167774E-13
 -0.11047887E+06-0.27469025E+02 0.62515193E+00 0.21534592E-01-0.21632848E-04
 0.80420186E-08-0.10761102E-12-0.10953325E+06-0.33231325E+01
 SIO2 J 9/67SI 1.0 2.00 0.00 0.G 300.000 5000.000
 0.58620396E+01 0.17719783E-02-0.75194197E-06 0.14180584E-09-0.98856402E-14
 -0.38767816E+05-0.68603497E+01 0.32628059E+01 0.85016601E-02-0.57388143E-05
 0.12896573E-10 0.97544976E-12-0.38035973E+05 0.66549120E+01
 SIS J12/71SI 1.S 1. 0. 0.G 300.000 5000.000
 0.41735773E+01 0.39282604E-03-0.15005173E-06 0.23242561E-10-0.60568870E-15
 0.11417754E+05 0.28555698E+01 0.28430691E+01 0.51150285E-02-0.63316074E-05
 0.34387326E-08-0.62623387E-12 0.11718930E+05 0.94328794E+01
 SI2 J 3/67SI 2.00 2.00 0.00 0.G 300.000 5000.000
 0.50474138E+01 0.53990027E-03-0.43078376E-06 0.11355206E-09-0.96262855E-14
 0.69133187E+05-0.19234581E+01 0.38155394E+01-0.19096542E-03 0.59233416E-05
 -0.57649601E-08 0.14775004E-11 0.69784625E+05 0.57275553E+01
 SI2C J 3/67SI 2.C 1.00 0.00 0.G 300.000 5000.000
 0.62510986E+01 0.13224175E-02-0.72805216E-06 0.23269424E-09-0.23285149E-13
 0.62301000E+05-0.72966413E+01 0.40438938E+01 0.73456950E-02-0.66412549E-05
 0.24885047E-08-0.18196555E-12 0.62935418E+05 0.41712494E+01
 SI2N J 3/67SI 2.N 1.00 0.00 0.G 300.000 5000.000
 0.66709909E+01 0.91917883E-03-0.39517130E-06 0.74397141E-10-0.50284687E-14
 0.45620152E+05-0.78114414E+01 0.36686735E+01 0.11301842E-01-0.13637119E-04
 0.71688042E-08-0.12378310E-11 0.46318082E+05 0.71095457E+01
 SI3 J 3/67SI 3.00 0.00 0.00 0.G 300.000 5000.000
 0.74213362E+01-0.11709948E-03 0.89820787E-07 0.71935964E-11-0.25670837E-14
 0.74146687E+05-0.10365274E+02 0.45979128E+01 0.10715272E-01-0.16100428E-04
 0.10969206E-07-0.27832875E-11 0.74766312E+05 0.34421673E+01
 SR(S) J12/70SR 1. 0. 0. 0.S 300.000 1041.000
 0.44565866E+01 0.82744707E-04 0.26667937E-07-0.17739116E-10-0.19199442E-13
 -0.16161782E+04-0.19842178E+02 0.14736900E+01 0.12286175E-01-0.32746320E-04
 0.44473232E-07-0.20957708E-10-0.74570654E+03-0.46496849E+01
 SR(L) J12/70SR 1. 0. 0. 0.I 1041.000 5000.000
 0.42271271E+01 0.0 0.0 0.0 0.0 0.0
 -0.34602051E+03-0.17212143E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 SR J12/70SR 1. 0. 0. 0.G 300.000 5000.000
 0.13790656E+01 0.25695092E-02-0.19999206E-05 0.60389804E-09-0.52548030E-13
 0.19343578E+05 0.11530002E+02 0.24997091E+01 0.20420084E-05-0.50245674E-08
 0.51744919E-11-0.18986000E-14 0.18981250E+05 0.55457878E+01
 SRCI J12/72SR 1.CL 1. 0. 0.G 300.000 5000.000
 0.43344421E+01 0.38952101E-03-0.24461315E-06 0.73284365E-10-0.59733339E-14
 -0.16208781E+05 0.55120964E+01 0.39036188E+01 0.24634427E-02-0.38776961E-05
 0.28303375E-08-0.77304119E-12-0.16139738E+05 0.75034876E+01
 SRCI2(S) J12/72SR 1.CI 2. 0. 0.S 300.000 1000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.69369631E+01 0.10787599E-01-0.13907940E-04
 0.58982259E-08 0.30133326E-11-0.10212719E+06-0.28370880E+02
 SRCI2(S) J12/72SR 1.CI 2. 0. 0.S 1000.000 1147.000
 0.14794947E+02 0.0 0.0 0.0 0.0
 -0.10642750E+06-0.75376221E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 SRCI2(L) J12/72SR 1.CL 2. 0. 0.L 1147.000 5000.000
 0.12580737E+02 0.0 0.0 0.0 0.0
 -0.10193675E+06-0.58076355E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 SRCI2 J12/72SR 1.CL 2. 0. 0.G 300.000 5000.000
 0.68964357E+01 0.11788718E-03-0.51854080E-07 0.10048831E-10-0.71584343E-15
 -0.59006902E+05-0.13675060E+01 0.58907137E+01 0.44942796E-02-0.72989405E-05
 0.53588138E-08-0.14730630E-11-0.58816402E+05 0.34120932E+01

SRF J12/72SR 1.F 1. 0. 0.G 300.000 5000.000
 0.42457161E+01 0.46633580E-03-0.26925898E-06 0.73560075E-10-0.57213755E-14
 -0.36740301E+05 0.44529152E+01 0.32713947E+01 0.46213344E-02-0.69007747E-05
 0.47233577E-08-0.12046805E-11-0.36555629E+05 0.90938578E+01
 SRF+ J12/72SR 1.F 1.E -1. 0.G 300.000 5000.000
 0.56135521E+01-0.21810918E-02 0.12215251E-05-0.16332971E-09 0.32584508E-14
 0.21882141E+05-0.39145756E+01 0.31093788E+01 0.50270036E-02-0.72689336E-05
 0.47548490E-08-0.11683848E-11 0.22607203E+05 0.90609550E+01
 SRF2(S) J12/72SR 1.F 2. 0. 0.S 300.000 1750.000
 0.88747162E+02-0.16376507E+00 0.65196902E-04 0.43548393E-07-0.23673480E-10
 -0.17456125E+06-0.46934521E+03 0.52916212E+01 0.15537657E-01-0.19211904E-04
 0.74965243E-08 0.94000589E-12-0.14853050E+06-0.24089157E+02
 SRF2(L) J12/72SR 1.F 2. 0. 0.L 1750.000 5000.000
 0.11912951E+02 0.0 0.0 0.0 0.0
 -0.14642806E+06-0.58022842E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 SRF2 J12/72SR 1.F 2. 0. 0.G 300.000 5000.000
 0.67547894E+01 0.27761958E-03-0.12158876E-06 0.23478774E-10-0.16675192E-14
 -0.94233625E+05-0.36551170E+01 0.48135519E+01 0.83821602E-02-0.12999531E-04
 0.91354408E-08-0.23989881E-11-0.93850562E+05 0.56509171E+01
 SRI2 J 6/74SR 1.I 2. 0. 0.G 300.000 5000.000
 0.74603682E+01 0.45403474E-04-0.20093275E-07 0.39155502E-11-0.28030988E-15
 -0.35300332E+05-0.17219324E+01 0.70450411E+01 0.18841699E-02-0.31175150E-05
 0.23299391E-08-0.65232135E-12-0.35223012E+05 0.24465907E+00
 SRO(S) J12/72SR 1.0 1. 0. 0.S 300.000 2938.000
 0.56477938E+01 0.13154000E-02-0.27640414E-06 0.67308326E-10-0.65626351E-14
 -0.73037375E+05-0.26098358E+02 0.35631371E+01 0.92717856E-02-0.11646579E-04
 0.70851840E-08-0.15259903E-11-0.72591375E+05-0.15928796E+02
 SRO(L) J12/72SR 1.0 1. 0. 0.L 2938.000 5000.000
 0.80516710E+01 0.0 0.0 0.0 0.0
 -0.66734750E+05-0.39092941E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 SRO J 6/74SR 1.0 1. 0. 0.G 300.000 5000.000
 0.96403027E+01-0.11285149E-01 0.78842322E-05-0.19035877E-08 0.15146548E-12
 -0.47499492E+04-0.25811340E+02 0.27329998E+01 0.67399405E-02-0.10800485E-04
 0.81767944E-08-0.23619873E-11-0.26443574E+04 0.10488127E+02
 TA(S) J12/72TA 1. 0. 0. 0.S 300.000 3258.000
 0.33300409E+01-0.31776121E-03 0.56893771E-06-0.25771318E-09 0.52179550E-13
 -0.10396860E+04-0.14038120E+02 0.30445547E+01-0.10359432E-02 0.51150728E-05
 -0.63806063E-08 0.26326042E-11-0.89585010E+03-0.12225083E+02
 TA(L) J12/72TA 1. 0. 0. 0.L 3258.000 5000.000
 0.50322943E+01 0.0 0.0 0.0 0.0
 -0.74377319E+03-0.25974213E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 TA J12/72TA 1. 0. 0. 0.G 300.000 5000.000
 0.15109091E+01 0.27029500E-02-0.10705598E-05 0.20238854E-09-0.13970172E-13
 0.93517750E+05 0.12969543E+02 0.28381634E+01-0.27878564E-02 0.68973332E-05
 -0.45571760E-08 0.94125228E-12 0.93278812E+05 0.66557741E+01
 TAC(S) J12/73TA 1.C 1. 0. 0.S 300.000 4273.000
 0.50027056E+01 0.12849041E-02-0.17495938E-06 0.35245584E-10-0.26429260E-14
 -0.19020555E+05-0.24129684E+02 0.10249720E+01 0.17628621E-01-0.25515852E-04
 0.17313308E-07-0.43057858E-11-0.18226598E+05-0.50093126E+01
 TAC(L) J12/73TA 1.C 1. 0. 0.L 4273.000 5000.000
 0.80516710E+01 0.0 0.0 0.0 0.0
 -0.10103340E+05-0.42085541E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0 0.0
 TAC J12/73TA 1.0 1. 0. 0.G 300.000 5000.000
 0.34996605E+01 0.15112534E-02-0.65384580E-06 0.17784314E-09-0.16919405E-13
 0.21994152E+05 0.85137959E+01 0.29340105E+01 0.30592037E-02-0.19396366E-05

0.16288830E-09 0.30152535E-12 0.22154473E+05 0.11441483E+02
 TAO2 J12/73TA 1.0 2. 0. 0.G 300.000 5000.000
 0.59701672E+01 0.11792127E-02-0.56517410E-06 0.13113786E-09-0.10564435E-13
 -0.26169480E+05-0.10871611E+01 0.31803827E+01 0.94702803E-02-0.87346871E-05
 0.24522688E-08 0.33653419E-12-0.25451762E+05 0.13117190E+02
 TA205(S) J12/72TA 2.0 5. 0. 0.S 300.000 2058.000
 0.18473679E+02 0.34902433E-02 0.91156585E-06-0.11508288E-08 0.24702061E-12
 -0.25245912E+06-0.90733490E+02 0.10119942E+02 0.25537558E-01-0.16847349E-04
 0.34734077E-10 0.31268009E-11-0.25008175E+06-0.47310883E+02
 TA205(L) J12/72TA 2.0 5. 0. 0.L 2058.000 5000.000
 0.29187302E+02 0.0 0.0 0.0 0.0
 -0.25336244E+06-0.15857774E+03 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 TIO2(S) CH3/77TI 1.0 2. 0. 0.S 298.000 2100.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.84212313E+01 0.29107044E-03 0.65353123E-06
 -0.42199044E-09 0.77775134E-13-0.11648344E+06-0.42814896E+02
 TIO2(L) CH3/77TI 1.0 2. 0. 0.L 2100.00 4000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.80215092E+01 0.13339046E-01-0.15539863E-05
 -0.49200533E-09 0.90296802E-13-0.95109500E+05 0.64583603E+02
 TIO2 CH3/77TI 1.0 2. 0. 0.G 298.000 6000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.67205629E+01 0.16490566E-03-0.71504815E-07
 0.19343499E-10-0.13055410E-14-0.39121559E+05-0.78946314E+01
 V(S) J 6/73V 1. 0. 0. 0.S 300.000 2190.000
 0.27552118E+01 0.38294797E-03 0.85178567E-06-0.50914206E-09 0.12945103E-12
 -0.78775073E+03-0.12252801E+02 0.18744802E+01 0.64936988E-02-0.11984017E-04
 0.10610506E-07-0.33844151E-11-0.76093311E+03-0.86898556E+01
 V(L) J 6/73V 1. 0. 0. 0.L 2190.000 5000.000
 0.55571632E+01 0.0 0.0 0.0 0.0
 -0.18994900E+04-0.30706696E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 V J 6/73V 1. 0. 0. 0.G 300.000 5000.000
 0.29177856E+01 0.46236883E-03-0.49732029E-06 0.16775233E-09-0.15202551E-13
 0.61064273E+05 0.50930519E+01 0.45173693E+01-0.79290643E-02 0.13380839E-04
 -0.88282910E-08 0.18945305E-11 0.60901418E+05-0.19828806E+01
 VCL2(S) L 3/74V 1.CL 2. 0. 0.S 300.000 1300.000
 0.95842199E+01-0.67106611E-03 0.84464722E-06 0.65502004E-09-0.39905741E-12
 -0.57330961E+05-0.43117737E+02 0.70783281E+01 0.80272816E-02-0.10977629E-04
 0.81348048E-08-0.22490213E-11-0.56733437E+05-0.30625641E+02
 VCL3(S) L 3/74V 1.CL 3. 0. 0.S 300.000 1000.000
 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.77660332E+01 0.17813500E-01-0.26194437E-04
 0.19483036E-07-0.54107656E-11-0.72758625E+05-0.32800827E+02
 VCL4(L) L 3/74V 1.CL 4. 0. 0.L 300.000 2000.000
 0.17415222E+02 0.13107814E-03-0.13408226E-06 0.59561092E-10-0.97181818E-14
 -0.73682812E+05-0.68552704E+02 0.17450150E+02 0.85973181E-04-0.21718432E-06
 0.22954140E-09-0.86409395E-13-0.73694625E+05-0.68744736E+02
 VCL4 L 3/74V 1.CL 4. 0. 0.G 300.000 5000.000
 0.12712587E+02 0.28488023E-04 0.13403843E-06-0.32849085E-10 0.21231135E-14
 -0.67185812E+05-0.28828003E+02 0.79819899E+01 0.19140452E-01-0.29540548E-04
 0.20644435E-07-0.53819440E-11-0.66212187E+05-0.59712782E+01
 VN(S) J12/73N 1.V 1. 0. 0.S 300.000 3500.000
 0.48368740E+01 0.18900146E-02-0.31610460E-06 0.46050663E-10-0.19102037E-14
 -0.27738152E+05-0.23873352E+02 0.81271356E+00 0.20101044E-01-0.31178002E-04
 0.23103688E-07-0.63845144E-11-0.27020094E+05-0.49457436E+01
 VN J12/73V 1.N 1. 0. 0.G 300.000 5000.000
 0.41852283E+01 0.61514718E-03-0.35776333E-06 0.10748862E-09-0.97275500E-14

0.61511539E+05 0.37630224E+01 0.27233591E+01 0.41642971E-02-0.21912811E-05
 -0.12351873E-08 0.10791836E-11 0.61927895E+05 0.11404194E+02
 VC(S) J12/73V 1.0 1. 0. 0.S 300.000 2063.000
 0.53398714E+01 0.17591703E-02 0.38477617E-06-0.26182478E-09 0.51009395E-13
 -0.53651379E+05-0.26382370E+02 0.25380402E+01 0.16447078E-01-0.28559807E-04
 0.24836392E-07-0.79886948E-11-0.53211918E+05-0.13599758E+02
 VC(L) J12/73V 1.0 1. 0. 0.L 2063.000 5000.000
 0.75484419E+01 0.0 0.0 0.0 0.0 0.0
 -0.47600473E+05-0.36154221E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 VO J12/73V 1.0 1. 0. 0.G 300.000 5000.000
 0.39114704E+01 0.77547785E-03-0.42263787E-06 0.11608838E-09-0.10070724E-13
 0.14065203E+05 0.50586910E+01 0.29438438E+01 0.29059234E-02-0.99516546E-06
 -0.14086592E-08 0.92438470E-12 0.14352746E+05 0.10173268E+02
 VO2 J12/73V 1.0 2. 0. 0.G 300.000 5000.000
 0.59470148E+01 0.11686778E-02-0.50536380E-06 0.96723615E-10-0.68245885E-14
 -0.29983801E+05-0.27511883E+01 0.31937857E+01 0.92979446E-02-0.83422465E-05
 C.21049169E-08 0.44582643E-12-0.29275492E+05 0.11274056E+02
 V203(S) J12/73V 2.0 3. 0. 0.S 300.000 2340.000
 0.13964211E+02 0.16871297E-02 0.11371203E-05-0.20806007E-09 0.10028325E-13
 -0.15100575E+06-0.68792898E+02 0.22877035E+01 0.57632763E-01-0.96738557E-04
 0.74066918E-07-0.20658392E-10-0.14911187E+06-0.14723446E+02
 V203(L) J12/73V 2.0 3. 0. 0.L 2340.000 5000.000
 0.18871109E+02 0.0 0.0 0.0 0.0 0.0
 -0.14034062E+06-0.94580917E+02 0.0 0.0 0.0 0.0
 0.0 0.0 0.0 0.0
 V204(S) J 3/77V 2.0 4. 0. 0.S 400.000 1800.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.15850223E+02 0.35800026E-02 0.61354478E-06
 -0.99711905E-09-0.27309399E-12-0.17577106E+06-0.76581085E+02
 V204(L) J13/77V 2.0 4. 0. 0.L 1800.000 3000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.28297012E+02-0.29605383E-02 0.11003967E-05
 -0.13310168E-09-0.76340581E-15-0.17637581E+06-0.15249167E+03
 V205(S) J 6/73V 2.0 5. 0. 0.S 300.000 943.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.11640358E+01 0.93535900E-01-0.15675098E-03
 0.12223524E-06-0.35738842E-10-0.18914531E+06 0.40722752E+00
 V205(L) J 6/73V 2.0 5. 0. 0.L 943.000 5000.000
 0.22947266E+02 0.0 0.0 0.0 0.0 0.0
 -0.18751450E+06-0.11089278E+03 0.22947266E+02 0.0 0.0
 0.0 0.0 -0.18751450E+06-0.11089278E+03
 W(S) J11/76W 1.0 0.0 0.0 0.S 298.000 3680.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 -0.25968343E+00 0.42470247E-02-0.94693121E-06
 -0.28325076E-09 0.10638333E-12 0.79613794E+03 0.58423100E+01
 W(L) J11/76W 1.0 0.0 0.0 0.L 3680.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.20796646E+02-0.74830465E-02 0.71120195E-06
 0.85091031E-10-0.12050802E-13-0.21700352E+05-0.13469987E+03
 W J11/76W 1.0 0.0 0.0 0.G 298.000 6000.000
 0.0 0.0 0.0 0.0 0.0 0.0
 0.0 0.0 0.37831755E+01-0.26602857E-03-0.97317283E-08
 0.38749920E-10-0.40930021E-14 0.10260281E+06 0.18369812E+00
 XE L 4/70XE 1.0 0.0 0.0 0.G 300.000 5000.000
 0.25000000E+01 0.0 0.0 0.0 0.0 0.0
 -0.74537500E+03 0.61512737E+01 0.25000000E+01 0.0 0.0
 0.0 0.0 -0.74537500E+03 0.61512737E+01
 END 0. 0. 0. 0. 0. 0.0

Appendix D**SAMPLE PROBLEMS**

Sample Problem 1: The Iron-Nickel System

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)	Z ENERGY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	NI 1.00000	0.00010	0.0		0.0	0.0
FUEL	FE 1.00000	0.00189	0.0		0.0	0.0
FUEL	H 1.00000	0.99801	0.0		0.0	0.0

O/F = 0.0 PERCENT FUEL=100.0000 EQUIVALENCE RATIO= 0.0 REACTANT DENSITY= 0.0

THERMODYNAMIC PROPERTIES

P, ATM	1.0000	0	1.0000	0	1.0000	0	1.0000	C	1.0000	0	1.0000	0	1.0000	0	1.0000	0	1.0000	0	1.0000	0	1.0000	0	1.0000	0		
T, DEG K	1700		1690		1680		1670		1660		1650		1640		1630		1620		1610		1600		1590		1580	
RHO, G/CC	1.4479-5		1.4565-5		1.4652-5		1.4740-5		1.4829-5		1.4919-5		1.5010-5		1.5102-5		1.5195-5		1.5290-5		1.5385-5		1.5482-5		1.5580-5	
H, CAL/G	5075.9		5036.4		4996.9		4957.5		4918.2		4879.0		4839.9		4800.8		4751.7		4722.8		4683.9		4645.0		4606.3	
S, CAL/(G) (K)	21.6393		21.6160		21.5925		21.5690		21.5454		21.5217		21.4979		21.4740		21.4500		21.4259		21.4016		21.3773		21.3528	
M, MOL WT	2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020		2.020	
(DLV/DLP)T	-1.00004		-1.00004		-1.00003		-1.00003		-1.00002		-1.00002		-1.00002		-1.00002		-1.00002		-1.00001		-1.00001		-1.00001		-1.00001	
(DLV/DLT)P	1.0014		1.0012		1.0011		1.0010		1.0009		1.0008		1.0007		1.0007		1.0006		1.0005		1.0005		1.0004		1.3004	
CP, CAL/(G) (K)	3.9590		3.9507		3.9427		3.9350		3.9275		3.9203		3.9133		3.9064		3.8993		3.8933		3.8869		3.8807		3.8746	
GAMMA (S)	1.3318		1.3326		1.3334		1.3342		1.3350		1.3357		1.3365		1.3372		1.3379		1.3386		1.3393		1.3400		1.3406	
SON VEL,M/SEC	3052.8		3044.8		3036.6		3028.5		3020.4		3012.0		3003.7		2995.3		2986.9		2978.4		2969.9		2961.4		2952.8	

MOLE FRACTIONS

FE(S)	6.2731-5	6.3601-5	6.4346-5	6.4987-5	6.5533-5	6.5998-5	6.6394-5	6.6730-5	6.7015-5	6.7255-5	6.7458-5	6.7628-5	6.7771-5											
FE	5.7200-6	4.8504-6	4.1044-6	3.4657-6	2.9201-6	2.4550-6	2.0594-6	1.7236-6	1.4393-6	1.1991-6	9.9653-7	8.2621-7	6.8330-7											
H	1.4639-4	1.3319-4	1.2105-4	1.0989-4	9.9646-5	9.0252-5	8.1646-5	7.3772-5	6.6574-5	6.0004-5	5.4013-5	4.8557-5	4.3594-5											
H2	9.9978-1	9.9980-1	9.9981-1	9.9982-1	9.9983-1	9.9984-1	9.9985-1	9.9995-1	9.9936-1	9.9987-1	9.9997-1	9.9988-1	9.9933-1											
NI(S)	3.3806-6	3.4029-6	3.4216-6	3.4374-6	3.4505-6	3.4615-6	3.4737-6	3.4784-6	3.4349-6	3.4902-6	3.4946-6	3.4983-6	3.5014-6											
NI	1.3422-7	1.1192-7	9.3210-8	7.7525-8	6.4383-8	5.3382-8	4.4193-8	3.6501-8	3.0095-8	2.4761-8	2.0329-8	1.6652-8	1.3608-8											

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOS MOLE FRACTIONS WERE LESS THAN 0.5000E-07 FOR ALL ASSIGNED CONDITIONS

FE(S) FE(L) FE(L) NI(L)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

NO INPT2 VALUE GIVEN FOR OP, EORAT, FA, OR FPCF

SPECIES BEING CONSIDERED IN THIS SYSTEM

J 3/65 FE(S) J 3/65 FE(S) J 3/65 FE(S) J 3/65 FE(S)
 H 6/76 H 3/61 H2 H 10/76 NI(S) H 10/76 NI(L) H 10/76 NI(E)

SELECTED COMPONENTS FOR SOLUTION PHASE ARE: Fe(s) Ni(s)

OF = 0.0	EFFECTIVE FUEL HPP(2)	EFFECTIVE OXIDANT HPP(1)	MIXTURE HSUBD
ENTHALPY (KG-MOL) (DEG K)/KG	0.0	0.0	0.0
KG-ATOMS/KG	BOP(I,2)	BOP(I,1)	B0(I)
NI	0.17402845E-05	0.0	0.17402845E-05
FE	0.33892196E-04	0.0	0.33892196E-04
HE	0.99011374E+00	0.0	0.99011374E+00

PT	NI	FE	H	
1	-6.708	-4.510	-9.480	14.303
1	-9.973	-6.992	-9.480	5.000
2	-9.961	-6.970	-9.471	2.000
3	-9.947	-6.947	-9.462	2.000
4	-9.932	-6.924	-9.453	2.000
5	-9.917	-6.900	-9.444	2.000
6	-9.901	-6.877	-9.435	2.000
7	-9.884	-6.854	-9.426	2.000
8	-9.867	-6.831	-9.417	2.000
9	-9.849	-6.807	-9.408	2.000
10	-9.831	-6.784	-9.399	2.000
11	-9.813	-6.760	-9.389	2.000
12	-9.794	-6.737	-9.380	2.000
13	-9.775	-6.713	-9.371	2.000

Sample Problem 2: The Potassium Oxide-Silica

THERMODYNAMIC EQUILIBRIUM PROPERTIES AT ASSIGNED

TEMPERATURE AND PRESSURE

	CHEMICAL FORMULA			MOLES	ENERGY	STATE	TEMP	DENSITY
	K	2.00000	O	1.00000	CAL/MOL	DEG K	G/CC	
FUEL	SI	1.00000	O	2.00000	0.30000	0.0	0.0	0.0
FUEL	AR	1.00000			0.70000	0.0	0.0	0.0

O/F = 0.0

PERCENT FUEL=100.0000

EQUIVALENCE RATIO= 1.0000

REACTANT DENSITY= 0.0

THERMODYNAMIC PROPERTIES

P, ATM	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2	1.0000-2
T, DEG K	1900	1800	1700	1600	1500	1400	1300	1200	1100	1000	900	800
RHO, G/CC	6.6064-6	7.2422-6	7.8171-6	8.3708-6	8.9515-6	9.5972-6	1.0337-5	1.1198-5	1.2217-5	1.3438-5	1.4931-5	1.6798-5
H, CAL/G	89.0	74.8	65.7	59.4	54.3	49.7	45.1	40.6	36.1	31.6	27.1	22.6
S, CAL/(G) (K)	0.9967	0.9716	0.9517	0.9347	0.9185	0.9019	0.8843	0.8653	0.8445	0.8217	0.7959	0.7672
M, MOLE WT	102.998	106.968	109.044	109.900	110.179	110.251	110.266	110.268	110.268	110.268	110.268	110.268
(DLV/DLPT)	-1.05331	-1.02641	-1.01051	-1.00328	-1.00081	-1.00016	-1.00032	-1.00000	-1.00000	-1.00000	-1.00000	-1.00000
(DLV/DLT)P	1.3721	1.1694	1.0778	1.0252	1.0065	1.0013	1.0002	1.0000	1.0000	1.0000	1.0000	1.0000
CP, CAL/(G) (K)	0.2836	0.2600	0.2460	0.2394	0.2372	0.2368	0.2372	0.2380	0.2390	0.2403	0.2461	0.2394
Gamma (S)	1.0808	1.0807	1.0817	1.0824	1.0825	1.0824	1.0822	1.0819	1.0816	1.0811	1.0732	1.0814
SON VEL,M/SEC	407.1	388.8	374.5	362.0	350.0	338.1	325.7	312.9	299.5	285.5	270.6	255.4

MOLE FRACTIONS

AR	6.6722-1	6.9291-1	7.0636-1	7.1190-1	7.1371-1	7.1417-1	7.1427-1	7.1428-1	7.1428-1	7.1428-1	7.1428-1	7.1428-1
K	3.7534-2	1.7063-2	6.3365-3	1.9073-3	4.6487-4	9.0159-5	1.3520-5	1.8708-6	1.7599-6	1.4901-6	1.4671-6	1.4671-6
KO	7.181	-5.2350	-5.715	-6.1022	-6.1343	-7.1262	-8.7849-10	2.297-11	3.402-14	1.385-17	7.407-22	2.868-27
K2	7.163	-8.1792	-8.3059	-9.3522-10	2.743-11	1.406-12	4.512-14	1.307-15	1.884-15	2.420-15	4.771-15	1.154-14
K2Si205(L)	1.8136-1	1.9933-1	2.0874-1	2.1262-1	2.1388-1	2.1421-1	2.1427-1	2.1428-1	2.1428-1	2.1428-1	2.1428-1	2.1428-1
O	2.409	-4.6.642	-5.1.489	-5.2.654	-6.3.061	-7.3.740	-8.2.578	-9.6.739-11	8.994-15	2.246-19	3.299-25	1.410-32
O2	6.247	-3.4.226	-3.1.575	-3.4.749	-4.1.156	-4.2.215	-5.3.013	-6.1.026	-7.1.843-13	2.896-20	5.328-29	0.0
SiO	3.940	-6.3.074	-7.2.053	-8.1.096	-9.4.198-11	1.034-12	1.494-14	1.781-16	9.457-17	3.910-17	2.106-17	1.138-17
SiO2(S)	1.0432-1	8.6377-2	7.6978-2	7.3098-2	7.1835-2	7.1507-2	7.1440-2	7.1430-2	7.1430-2	7.1430-2	7.1430-2	7.1430-2
SiO2	1.036	-6.1.096	-7.9.752	-9.6.891-10	3.541-11	1.201-12	2.409-14	2.498-16	1.117-18	1.670-21	5.791-25	2.688-29

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 0.50000E-37 FOR ALL ASSIGNED CONDITIONS

K(S)	K(L)	K2O(S)	K2O(L)	O3	Si(S)	Si(L)	Si	SiO2(S)	SiO2(S)
SiO2(L)	Si2	Si3							

NO INPT2 VALUE GIVEN FOR OP. FOBAT, FA, OR FRCT

SPECIES BEING CONSIDERED IN THIS SYSTEM

L 5/66 BR J12/61 K(S) J12/61 K(L) J 6/62 K J12/67 KO
 J12/61 K2 J 6/63 K20(S) H10/77 K20(L) PB7/77 K2SI205(L) J 6/74 O
 J 9/65 O2 J 6/61 03 J 3/67 SI(S) J 3/67 SI(L) J 3/67 SI
 J 9/67 SI0 J 6/67 SI02(S) J 6/67 SI02(S) J 6/67 SI02(S) J 6/67 SI02(L)
 J 9/67 ST02 J 3/67 ST2 J 3/67 ST2

SELECTED COMPONENTS FOR SOLUTION PHASE ARE: K2Si2O5(L) SiO2(S)

$$\Omega F = 9.9$$

EFFECTIVE FUEL		EFFECTIVE OXIDANT		MIXTURE
	HPP(2)		HPP(1)	HSUB0
ENTHALPY (KG-MOL) (DEG K)/FG	0.0		0.0	0.0
KG-ATOMS/RG	BOP(I,2)		BOP(I,1)	BO(I)
K	0.54412670E-02		0.0	0.54412670E-
O	0.15416913E-01		0.0	0.15416913E-
SI	0.63481443E-02		0.0	0.63481443E-
AR	0.90687834E-02		0.0	0.90687834E-

PI	K	O	SI	AR	
1	-22.243	-17.615	-24.739	-26.709	11.000
1	-23.701	-18.761	-33.770	-25.806	7.000
2	-24.062	-19.059	-36.185	-25.655	4.000
3	-24.584	-19.454	-38.690	-25.517	4.000
4	-25.266	-19.952	-41.359	-25.385	4.000
5	-26.101	-20.552	-44.306	-25.252	3.000
6	-27.033	-21.268	-47.642	-25.114	3.000
7	-28.257	-22.149	-51.423	-24.970	3.000

8	-29.395	-23.718	-54.808	-24.818	3.000
9	-28.483	-30.205	-49.605	-24.656	3.000
10	-27.504	-37.905	-43.611	-24.486	1.000
11	-26.147	-47.822	-35.366	-24.305	2.000
12	-24.467	-60.433	-24.745	-24.114	2.000
13	-22.352	-76.858	-19.816	-23.914	2.000

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